IDENTIFICATION OF HAZARDOUS MOTOR VEHICLE ACCIDENT SITES: SOME BAYESIAN CONSIDERATIONS

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Abstract

Appropriate hazardous accident site identification and discrimination is a fundamental difficulty that confronts traffic safety researchers. Readily employed Bayesian methods can redress this difficulty and are the focus of this thesis.

Accident analysis, including hazardous site identification, invariably requires the specification of some defined distributional function. However, several different distributions have been proposed to model traffic accidents, and so the most suitable model amongst these must be appropriately determined and selected.

Model selection should satisfactorily fulfill two requisite criteria; firstly, that the *best* model is discriminated, and secondly, that this best distribution *adequately* describes the data. To help satisfy these requirements we introduce the *averaged Bayes factor*, a new method that determines the *best* model from likely candidate distributions, and we propose a new Bayesian procedure that facilitates the quantitative assessment of model *adequacy*. In addition, a method quantifying the *power* of detecting model inadequacy is presented.

With the specification of an appropriate accident distribution, procedures facilitating hazardous site identification, ranking and selection are then proposed. These procedures are accomplished using the hierarchical Bayesian method and three intuitive quantitative strategies. Especially useful is a variation of the posterior probability that gives the probability each particular site is worst and by how much it is worst. All proposed techniques are illustrated using previously published accident data from 35 sites in Auckland, New Zealand.

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Chapter 1

Introduction

1.1 Background

Internationally, Trinca *et al.* (1988) opine, at least half a million people are killed and 15 million are injured annually due to motor vehicle accidents. New Zealand, between the years 1951–1992, officially recorded 23,548 road fatalities and 657,581 road injury accidents for a population that expanded from 2.0 to 3.5 million (New Zealand Land Transport Safety Authority, 1992). Clearly the subject of motor vehicle accidents is of immense social importance and demands thorough scientific investigation by researchers in a variety of fields.

Correction of hazardous sites is one avenue available to traffic engineers in their endeavour to reduce future accident numbers. Typical procedures for hazardous site correction involves three basic tasks:

1. identification of hazardous locations;
2. diagnosis of the problems at identified locations and determination of potential remedial treatments; and
3. appraisal of alternative treatments (to identify the most cost-effective) followed

by implementation of the best treatment if sufficiently cost-effective.

The first and most fundamental task of hazardous site identification is the primary focus of the research described in this thesis.

Customarily, determination of those locations which appear unusually hazardous is accomplished by comparing accident numbers, recorded over a common period, at some collection of sites. Such comparisons and subsequent analytical investigations have traditionally been made on the assumption that accident occurrence is governed by the Poisson distribution.

1.2 The Poisson assumption

Gerlough and Schuhl (1955) were one of the first to formalise the use of the Poisson distribution in the literature on traffic accident estimation and accident site comparison. Since this time a succession of authors, most prominently Haight (1967), have continued in a similar vein and assumed Poisson accident occurrence in any theoretical development. However, until recently, there has been scant empirical research specifically investigating and validating the appropriateness of this assumption.

While the Poisson model is appealing, in that only one parameter requires estimation, it is also restrictive, in the sense that the theoretical *dispersion index* (variance to mean ratio) must equal unity. To be consistent with this theoretical constraint, accident data should yield empirical dispersion indices that are centred around unity. Instances arise, however, where empirical dispersion indices are considerably discrepant from unity, thereby casting doubt upon the appropriateness of the Poisson distribution.

Some of the dispute concerning the validity of the Poisson assumption has centered on the data tabulated within Appendix A and analysed within this thesis. Initially, Nicholson (1985), using an approximate test, suggested this data exhibited more variation in the empirical dispersion index than could be expected from the Poisson assumption. He concluded that the Poisson density may not always be appropriate. Later, Nicholson and Wong (1993) using these same data but an exact combinatorial method, gleaned from Fisher (1950), recanted by concluding that the Poisson distribution was generally suitable.

Other authors (Hutchinson and Mayne, 1977, Hauer 1978, Hauer, 1986, Hauer,

Ng and Lovell, 1988), using alternative accident data, have observed that the Poisson distribution alone was not the most suitable model. This disenchantment with the Poisson model has primarily stemmed from anecdotal evidence[1] produced by a variety of investigators describing that, in many instances, the empirical variance is greater than the observed mean. Frequently, the associated empirical variance has reportedly been appreciably greater than the observed mean.

Instead the negative binomial distribution, derived from a gamma mix of Poisson parameters, has been favoured by many to account for the extra variability frequently associated with traffic accident data. Given this genesis of the negative binomial distribution, we refer to it hereafter as the Poisson/gamma density.

The uncertainty in the Poisson assumption for modelling accidents is not a recent phenomenon. In 1898, Bortkiewicz (Johnson and Kotz, 1969) satisfactorily fitted a Poisson distribution to the annual number of soldiers dying from mule kicks in the Prussian Army Corps. However, two decades later, Greenwood and Yule (1920) observed that the Poisson/gamma distribution more closely fitted those data than did the Poisson. But as these authors pointed out, closeness of fit is not proof that the underlying hypothesis is correct. Nonetheless, a decision must be made as to which probability generating function should be employed; a decision frequently made in an intuitive but *ad hoc* unsophisticated way.

1.3 Model selection

Selection of an appropriate distribution from a collection of likely candidate models requires the satisfactory fulfillment of two fundamental criteria; namely, which among the group of candidates is *best* and is this best distribution *adequate*?

Goodness-of-fit tests and methods based on likelihood ratio criteria have traditionally been used by frequentist statisticians to compare and choose between competing models (see D'Agostino and Stephens, 1986, or Agresti, 1990, for example). Assuming that the model under consideration is true, goodness-of-fit tests are based on calculating the tail area probability associated with a selected measure of

[1]Anecdotal in the sense that scant statistical evidence has been furnished in the traffic literature either vindicating or admonishing the general applicability of the Poisson model.

discrepancy to assess whether evidence exists to determine if the model is incompatible with the observed data. Three commonly employed discrepancy measures are the chi-square, likelihood-ratio and Kolmogorov-Smirnov statistics. These frequentist methods, then, address both fundamental criteria simultaneously. However, important companion power computations are frequently lacking and hence these tests alone are of dubious value.

Current Bayesian model selection techniques do not simultaneously address the two fundamental criteria. Instead, discrimination is initially made between the competing models followed by an assessment of the adequacy of the most likely model in representing the data (Rubin, 1984, Gelman *et al.*, 1995). Compared to the frequentist approach, some may consider this two stage Bayesian approach cumbersome or inconvenient. We make no apology for the Bayesian approach as the inherent advantages of this paradigm, we believe, outweigh the serious limitations contained within the traditional frequentist methods. While it is not our endeavour, in this thesis, to formally survey and critique frequentist methods, it should nevertheless be re-emphasised that these methods can not embody expert prior information into their estimation framework and they rely upon tests of hypotheses to assess differences between accident sites. In the accident analysis framework, these deficiencies are quite unsatisfactory.

Section 1.3.1 introduces discrimination methodologies that facilitates identification of *best* models, while Section 1.3.2 introduces techniques allowing determination of model *adequacy*. With the adoption of these techniques, the aforementioned uncertainty in the appropriateness of the Poisson density can be quantifiably assessed.

1.3.1 Discrimination

Discrimination between a group of competing models and determination of the *best* model within the given group is commonly made, in the Bayesian framework, using the Bayes factor; an excellent review and summary of Bayes factors is provided by Kass and Raftery (1995).

When discriminating between a multiple of candidate models at a collection of accident sites, it is unrealistic to expect that sufficient expert information will always be available to specify proper prior distributions so that the standard Bayes factor pair-wise model comparisons can be made. In these circumstances, the adoption

of noninformative priors would more appropriately reflect the quantity (or quality) of expert information available to the analyst. However, appropriately defined noninformative priors are invariably improper, in that they have infinite mass.

It is well documented that should improper noninformative priors be adopted then ensuing Bayes factors are only defined up to an unspecified ratio (O'Hagan, 1995, Berger and Pericchi, 1996), thereby negating their usefulness for selection purposes. However, the appeal of the Bayes factor has compelled a succession of authors to develop strategies that enable its computation in the absence of prior information. Approximations to the Bayes factor, such as the Bayesian information criterion (BIC) introduced by Schwarz (1978), or the implementation of conventional proper prior distributions, despite the unavailability of prior information, have historically been the most readily adopted methods. While the BIC technique is generally easy to compute, this criterion contains several fundamental deficiencies, particularly for selection based upon small sample numbers. Alternatively, specification of proper prior distributions in the event where, at most, only vague prior information exists is difficult to justify and not well suited for selection between multiple models of varying or large dimension.

Recently, several techniques facilitating the use of improper noninformative priors for Bayes factor derivations have been contributed to the literature. These techniques frequently rely on various forms of *training samples* and *partial likelihood methods*. For instance, Smith and Spiegelhalter (1980) and later Spiegelhalter and Smith (1982) use imaginary training samples; Aitkin (1991, 1992) uses the entire sample as a training sample and then uses the data again for determination of his Bayes factor; O'Hagan (1995) uses a fractional part of the likelihood density, instead of a training sample, to derive a Bayes factor; and, Berger and Pericchi (1996) take averages of Bàyes factors over all combination of minimal training samples.

These approaches have various weaknesses. Spiegelhalter and Smith remove the arbitrary normalising constants by conducting an experiment based upon a minimal set of imagined data. The concept of a minimal experiment is not precisely defined, leading to ambiguity over its definition and potentially producing quite discrepant results (see O'Hagan, 1995, and Aitkin, 1991, for more detailed discussion). It is Aitkin's repeated use of the entire sample, firstly as a training sample, and secondly, in calculation of his *posterior Bayes factor* that is inconsistent with

traditional Bayesian logic and that introduces bias (see discussants to Aitkin, 1991, and Berger and Pericchi, 1996). The *fractional Bayes factor* suggested by O'Hagan certainly warrants further investigation. Difficulty currently exists with this method in determining how large a fraction of the entire likelihood is required for accurate and stable estimates, particularly when sample sizes are small. Berger and Pericchi's *intrinsic Bayes factor* yields discrepant results for differing noninformative priors, produces factors that depend on the type of averaging employed, and potentially demands considerable numerical computation especially when there are numerous training samples or model comparisons.

In this thesis we present a new Bayesian technique, entitled the *averaged Bayes factor*, that is free from these limitations. Upon implementation, the *averaged Bayes factor* will enable practitioners to quantitatively and more accurately determine the most appropriate generating functions from a group of competing functions in the absence of prior information. One particular salient advantage of this technique, apposite to traffic accident analysis, is that model discrimination can be based upon a relatively small number of observations.

Once a *best* model has been discriminated from a group of competing densities, it is important to determine whether this model is consistent with the observed data. That is, in accordance with the second fundamental criterion, an assessment of the model's *adequacy* in representing its data is required.

1.3.2 Adequacy

It is well recognised that statistically defined distributional functions are merely convenient conceptual representations of observed phenomena and, apart from rare situations, any model specification will never be *correct*. The purpose of model selection, therefore, is to find those distributional functions that best or most closely represent the observed data and that are themselves consistent with this data.

Discrimination made from an incomplete list of candidate distributional functions or by using data that are either insufficient or of poor quality may result in the *best* models not representing their data *adequately*. To illustrate, suppose an entire set of competing models poorly represent some data. Implementation of a Bayes factor model discrimination strategy guarantees that the "best" distribution will be determined. This best distribution will be genuinely superior to its competitors but,

nonetheless, will remain inadequate at describing the empirical data. Should this *inadequate* distributional function nonetheless be employed for inferential purposes, then resultant answers could be seriously in error.

Model discrimination using *Bayes factors*, or some variant, make no explicit consideration of *model adequacy*. Indeed, when implemented, these discrimination strategies advocate, without fail, superior models from a group of candidates, regardless of their fit. Such Bayesian strategies, then, provide no assurance that selected models *adequately* describe their data. Only model selection, combined with diagnostics of model adequacy, will provide this assurance. Surprisingly, the topic of *model adequacy* does not appear to have received the attention it deserves in the Bayesian framework, although Rubin (1984), Draper *et al.* (1993), Upadhyahy and Smith (1993), and Gelman *et al.* (1995), amongst others, have all discussed the subject.

Box (1980) persuasively argues that model validation should result from the assessment of that model's predictive distribution and not from its posterior distribution of model parameters, particularly since prediction is the primary purpose of any chosen model. Berger (1985) concurs with this belief and notes that Bayesians have historically employed predictive distributions to validate assumptions. Based upon the predictive distribution and using cross-validatory techniques, Gelfand, Dey and Chang (1992) propose a set of adequacy measures (denoted here by $\mathcal{D}^r$) to scrutinise the ability of any model to mimic data. An addition to this list, using the full predictive distribution, is the Kolmogorov-Smirnov discrepancy measure, suggested by Upadhyahy and Smith (1993). Cross-validation essentially uses successive partitions of the data for determining the predictive distributions under each selected model, and then assesses adequacy by examining each model's performance in predicting the associated hold-out samples, using various adequacy measures. The full predictive method measures the discrepancy between the cumulative predictive distribution and the empirical cumulative frequency distribution, in the Kolmogorov-Smirnov fashion.

These adequacy measures, when evaluated on data for a given set of models, provide no easily interpretable information pertaining to the compatibility between models and the observed data. That is, the $\mathcal{D}^r$ adequacy measures, when numerically computed, yield measurements that in the absence of a *frame of reference*, do

not suggest whether any particular model is adequate or not. We need to know what sort of measurements could be expected if the model under consideration was indeed the underlying generating function. A model's adequacy could then be accepted or rejected by comparing the observed adequacy measure to its expected range. Clearly, if the observed adequacy measure falls within its expected range then no reason exists to dispute that model's adequacy; conversely, outlying observed adequacy measures cast doubt on the adequacy of the model under investigation.

Advances in computing capacity and numerical techniques enable development of the expected range to be viably ascertained through computer simulation. Computer simulation is a well established statistical tool, important and necessary for the determination of many intractable statistical problems. For example, Markov chain Monte Carlo (MCMC) approaches such as the Gibbs sampler (Gelfand and Smith, 1990), sampling–resampling techniques (Smith and Gelfand, 1992) and the Metropolis algorithm (Metropolis *et al.*, 1953, Hastings, 1970, Müller, 1991) have enabled statisticians to evaluate integrals rarely possible prior to the advent of this method. Applications of sophisticated Bayesian analysis are now routinely undertaken on a vast array of problems using these easily implemented simulation procedures.

In this thesis we propose a new method that facilitates the determination of a frame of reference for any suitable adequacy measure, such as those delineated in Gelfand, Dey and Chang (1992) and Upadhyahy and Smith (1993). Development of the reference frame uses methods in cross-validation (Geisser and Eddy, 1979), prediction (Box, 1980) and simulation (such as Smith and Roberts, 1993). Once this frame of reference has been derived, a quantitative assessment as to whether the data were likely to have originated from the selected model can be made. Several methods of assessment are described. Moreover, a natural extension of this approach allows the quantitative computation of *power*, the probability that a model is deemed inadequate when the data actually arise from some alternative model. This measurement of power provides the strength of the adequacy measures ability in detecting observations from alternative distributions. Equipped with these techniques, the second fundamental model selection criterion can be readily and appropriately addressed.

Upon specification of an appropriate accident distribution (one that satisfies both fundamental criteria) analyses identifying the most hazardous locations can

then ensue.

1.4 Ranking and selection

Traffic accidents occur with such rarity that long observation periods (such as annual intervals) are necessary to ensure that non-zero counts will be recorded. As an immediate consequence, accident analysis typically deals with diminutive sample sizes that yield estimated accident rates with large associated variance components. Tests of hypothesis employed to detect statistical differences between accident sites, then, have little power to discern such differences. This deficiency has impelled traffic accident analysts to consider alternative methods.

As a matter of expediency, hazardous accident locations are frequently identified using *ordered lists*. This can involve identifying some specified percentage of sites with the highest empirical accident rate (defined to be the summed observed accident count divided by the length of monitoring), but more commonly involves identifying those locations where the empirical accident rate exceeds some specified threshold. Whichever approach is adopted, it is common practise to prepare lists of accident locations, ordered according to their empirical accident rate.

The ordered list is important as locations are generally selected by working down the list until the allocated resources are exhausted for the detailed examination (that is the diagnosis and identification of potential treatments) and, perhaps, subsequent treatment of locations. Different list orderings may well lead to a different set of locations being examined in detail. An inappropriate ordering of locations, therefore, could lead to a truly hazardous location not being examined and considered for treatment.

Ordered lists constructed by ranking locations according to their empirical accident rate, ignoring the variability associated with each estimate, do not ensure that the worst location(s) will be identified. Moreover, selection based upon this ranking strategy provides no statement as to the probability that the worst location(s) has been selected nor, equally importantly, by how much it is worst. Alteratively, if one is comparing accident rates with threshold values then it is helpful to know the probabilities of particular sites having underlying accident rates exceeding some threshold. Although a particular site may have a high empirical accident rate, if its

period of observation is short compared to the other locations then this probability may be relatively small and thus it would be inappropriate to expend resources on (2), the diagnosis of problems and determination of potential remedial treatments for such a site, or (3), the appraisal of alternative treatments followed by implementation of the best treatment.

Bayesian methods have received increasing support from traffic researchers attempting to overcome these difficulties associated with the hazardous site identification problem; several recent Bayesian and empirical Bayesian papers dealing specifically with this problem ensue. Empirical Bayesian estimation procedures were explored by Hauer (1986) that enhanced the accuracy of empirical accident rate estimators. Higle and Witkowski (1988) specify an upper limit, $\bar{\lambda}$, on the 'acceptable' underlying accident rate, and identified a site i as being hazardous when the probability that the underlying accident rate exceeded $\bar{\lambda}$ by a predetermined tolerance level, δ. Davies (1990) proposed a procedure for ranking a set of entities by considering a ratio, p, between the underlying accident rate at each entity (target site) and the pooled underlying accident rates of the remaining entities (reference sites). For each target site a posterior distribution for p was derived and used to ascertain a similarity measure $\alpha = Pr(p < 1 \mid \text{ data })$. When the target site has a comparatively large underlying accident rate, compared to the reference group, most of the posterior mass for p exceeds 1. A small value of α, therefore, provided evidence that the target site had a higher underlying accident rate than the reference sites and formed the basis for selection.

Another form of the Bayesian approach, called the hierarchical Bayesian model, has received some limited attention in the traffic accident literature. Christiansen, Morris and Pendleton (1992) developed a hierarchical Bayesian Poisson regression model for both the estimation and ranking of accident sites. Their site selection criterion consisted of ranking, in descending order, the posterior accident rate estimates for each site modified by factors such as: installation cost; future traffic volume; and expected accident reduction if that site is modified. Sites were then selected sequentially from the ordered list until an overall budget allocation was met. A hierarchical Bayesian approach was also adopted by Ibrahim and Metcalfe (1993) in their evaluation of mini-roundabouts as a road safety measure. Adoption of this

model enabled these authors to easily combine data from different sources and different time periods so that an assessment of the effect of replacing priority-controlled junctions by mini-roundabouts could be made.

None of the above procedures deal with the problem of selecting a subset of accident sites based on a probability assertion that the worst sites are selected. Nor, perhaps more importantly, are any probability assertions made as to *how much worse* one site is compared to another. While methods facilitating such probabilistic assertions receive increasing attention in the literature (Gupta and Yang, 1985, Deely and Gupta, 1988, Berger and Deely, 1988, Fong, 1992, Fong and Berger, 1993, Fong, Chow and Albert, 1994), these techniques remain absent from current traffic accident analysis practice.

It is a primary purpose of this thesis, therefore, to address these serious and practically important inadequacies. In particular we describe the behaviour of three strategies that can be used to accomplish the above goals. As will be demonstrated, these selection criteria investigate different characteristics of the model and often result in different site rankings. One procedure, founded upon predictive probabilities, will have selection demonstrated using a new and easily implemented graphical technique.

Presented within each proposed selection criterion are two intuitively appealing procedures suitable for selecting subsets of hazardous sites. Adoption of a particular procedure depends on the practical requirement of the situation: should a subgroup with fixed size r be desired, then the r most hazardous sites can be easily ascertained; or should target safety levels be a primary focus, then selection of sites that exceed designated hazardous threshold values can be made. Selection based on a fixed subset size r will appeal to those with resource constraints while selection based upon target safety levels will appeal to those wanting to avoid potentially 'embarrassing' levels of future accidents.

It is generally unrealistic to assume (de Finetti, 1974) that prior information can be readily and reliably elicited for each *individual* site under investigation. We believe, in practice, expert prior information pertaining to the characteristics of the *grouping* of accident sites under investigation is both more readily available and reliable. This appealing feature is embodied in our model by assuming exchangeability amongst the underlying accident rates, which implies that these rates arise from

some common distribution. Based upon the exchangeability assumption, our proposed ranking and selection strategies parallel Bayesian considerations previously made on the normal means problem; in particular, by Berger and Deely (1988) and Fong and Berger (1993) to ANOVA models, by Fong (1992) to ANCOVA models, and, by Fong, Chow and Albert (1994) on selecting the largest regression value. Additionally, similar techniques have been employed to the binomial data problem by Deely and Gupta (1988).

1.5 Overview

Before appropriate identification of hazardous sites can be undertaken, at least in the Bayesian framework, specification of a statistical accident model is required. This thesis proposes and combines new techniques in *model discrimination* and *model adequacy* which facilitate the determination of such a model. Once the accident model is determined, procedures facilitating hazardous site *ranking* and *selection* will then be proffered.

Chapter 2 introduces four candidate accident models, derives their associated noninformative priors and details the relevant notation. It is from these four candidate models that model discrimination will be made, and this is the primary focus of Chapter 3. Preliminary statistical techniques necessary for the derivation of the *averaged Bayes factor* model discrimination method (such as the Bayes factor, training samples and partial likelihood techniques), are described in Section 3.1. This section also elucidates the problem encountered when employing improper noninformative priors to standard Bayes factor calculations. The averaged Bayes factor is then described and statistically presented in Section 3.2. Next, the frequently adopted approximation to the Bayesian information criterion (BIC) is briefly summarised and discussed in Section 3.3. Both discrimination techniques are employed in Section 3.4, where discrimination between the four competing models (introduced in Chapter 2) is conducted using previously published and discussed traffic accident data for 35 intersection sites in Auckland, New Zealand. These accident data appear in Table A.1 of Appendix A.

The adequacy of the discriminated models is the principle consideration of Chapter 4. Again, some preliminaries are required (defining posterior densities, posterior

predictive densities and hold-out predictive distributions) and these are found in Section 4.1. Three specific measures of model adequacy are introduced in Section 4.2 and procedures that facilitate their assessment and interpretation are given. The next section follows with the theoretical and numerical development of power calculations for these measures. A simulation technique that enables the determination of model adequacy and associated power is then introduced in Section 4.4. All these techniques are combined in Section 4.5 where adequacy analysis is conducted on the four candidate distributions using the same Auckland data.

Section 5.1 of Chapter 5 begins with a synthesis of the analyses contained within the preceding chapters and culminates with the identification of the most globally suitable candidate model so that ranking and selection strategies can be formulated. These ranking and selection strategies form the primary basis of Chapter 5. The theoretical development uses a hierarchical Bayesian model, and this is presented in Section 5.2. The proposed selection strategies are delineated in Section 5.3. Discussions concerned with prior information distributional form, elicitation and application to the model follow in Section 5.4. Numerical analyses using the accident data housed in Table A.1 ensue in Section 5.5. These analyses demonstrate aspects of the model and selection criteria proposed.

In each of the Chapters 3–5, helpful computation suggestions appear and a description of how the numerical calculations were undertaken for this thesis. Appendices B, C and D house tabulations of the numerical results derived from the implementation of the methods described in Chapters 3, 4 and 5, respectively.

Finally, Chapter 6 recapitulates the principle conclusions, discussions and provides direction for further research.

Chapter 2

Mathematical models and notation

2.1 Candidate distributions

Traffic accident analysis, including the identification of hazardous locations and the evaluation of treatment effectiveness, has traditionally been based on the assumption that observed accident occurrence can be adequately described by the Poisson distribution. This general model panacea is not, however, without question, particularly in those instances where the empirical dispersion index (variance to mean ratio) is considerably discrepant from unity. Instead, to accommodate the empirical over-dispersion commonly associated with traffic accident data, the Poisson/gamma distribution has been preferred by some investigators.

There are in fact a myriad of potential alternative densities. However, for the purpose of this thesis, four candidate densities are considered: namely, the incumbent Poisson distribution; the Poisson/gamma distribution (or negative binomial distribution, obtained from a gamma mix of Poisson parameters); the mixture of two Poisson densities; and the hitherto unused geometric density.

The consideration of these statistical distributions implies that, for a given site

and jth candidate distribution, independent accident data are assumed to be conditioned upon some vector of unknown parameters $\boldsymbol{\theta}_j$. If the conditionally independent accident data are recorded over some period n, denoted by $\boldsymbol{x} = (x_1, \ldots, x_n)$, then this assumption implies that X_i, the accident numbers recorded in the ith interval, can be potentially described by any of the four following models.

- M_1: a *Poisson distribution* given by

$$f_1(x_i \mid \boldsymbol{\theta}_1) = \frac{\lambda^{x_i} e^{-\lambda}}{x_i!} \tag{2.1}$$

where

$$\boldsymbol{\theta}_1 = \{\lambda\} \quad \text{with} \quad 0 < \lambda < \infty.$$

This distribution has mean and variance

$$\mathrm{E}_1[X_i] = \lambda \quad \text{and} \quad Var_1(X_i) = \lambda. \tag{2.2}$$

- M_2: *Poisson/gamma distribution* derived from the Poisson likelihood distribution,

$$f(x_i \mid \lambda_i) = \frac{\lambda_i^{x_i} e^{-\lambda_i}}{x_i!},$$

and the gamma prior distribution, assuming the λ_i's are i.i.d., given by

$$\pi(\lambda_i \mid a, p) = \left(\frac{p}{1-p}\right)^a \frac{\lambda_i^{a-1} e^{-\lambda_i p/(1-p)}}{\Gamma(a)},$$

then

$$\begin{aligned} f_2(x_i \mid \boldsymbol{\theta}_2) &= \int_0^\infty f(x_i \mid \lambda_i)\, \pi(\lambda_i \mid a, p)\, d\lambda_i \\ &= \binom{x_i + a - 1}{x_i} p^a (1-p)^{x_i} \end{aligned} \tag{2.3}$$

for

$$\boldsymbol{\theta}_2 = \{a, p\} \quad \text{with} \quad 0 < a < \infty \ \text{ and } \ 0 < p < 1.$$

Notice that (2.3) is negative binomial in distribution, thereby having mean and variance equal to

$$\mathrm{E}_2[X_i] = \frac{a(1-p)}{p} \quad \text{and} \quad Var_2(X_i) = \frac{a(1-p)}{p^2}. \tag{2.4}$$

- M_3: a *mixture of two Poisson densities* is defined by

$$f_3(x_i \mid \boldsymbol{\theta}_3) = p\frac{\lambda_1^{x_i} e^{-\lambda_1}}{x_i!} + (1-p)\frac{\lambda_2^{x_i} e^{-\lambda_2}}{x_i!} \tag{2.5}$$

where

$$\boldsymbol{\theta}_3 = \{p, \lambda_1, \lambda_2\} \quad \text{with} \quad 0 < p < 1 \ \text{ and } \ 0 < \lambda_1 < \lambda_2 < \infty.$$

Adopting standard statistical techniques it is straightforward to derive the mean and variance for this distribution; these quantities are given by

$$\begin{aligned} \mathrm{E}_3[X_i] &= p\lambda_1 + (1-p)\lambda_2 \quad \text{and} \\ Var_3(X_i) &= p(1-p)(\lambda_1 - \lambda_2)^2 + p\lambda_1 + (1-p)\lambda_2. \end{aligned} \tag{2.6}$$

- M_4: a *geometric distribution* with density function

$$f_4(x_i \mid \boldsymbol{\theta}_4) = p(1-p)^{x_i} \tag{2.7}$$

for

$$\boldsymbol{\theta}_4 = \{p\} \quad \text{with} \quad 0 < p < 1.$$

This geometric distribution has mean and variance of the form,

$$\mathrm{E}_4[X_i] = \frac{(1-p)}{p} \quad \text{and} \quad Var_4(X_i) = \frac{(1-p)}{p^2}. \tag{2.8}$$

The Poisson distribution, predominantly assumed as the underlying model in accident analysis, is constrained by the condition that the mean and variance are identical, as given by (2.2). Clearly, this equivalence in the mean and variance restricts the theoretical dispersion index to a single point at one. While the Poisson's simplicity is attractive, this constraint does appear restrictive at times.

The Poisson/gamma distribution is frequently a first choice alterative when it is opined that a Poisson distribution might be inappropriate (Johnson and Kotz, 1969). This is because the Poisson/gamma density has been recognised to often give an adequate representation of accident data when the strict randomness requirements of the Poisson distribution are not sufficiently met. Empirical over-dispersion has thus lead many researchers to entertain the Poisson/gamma model as an appropriate

alternative distribution for measuring traffic accident data. As can be seen from (2.4), this distribution has a variance greater than its mean, thereby allowing the theoretical dispersion index to range on the $(1, \infty)$ interval.

Density functions based on mixtures of distributions have received some attention in the statistical literature (Ashton, 1971, Everitt and Hand, 1981, Philippou, 1989). Indeed this type of approach seems particularly pertinent to the investigation of traffic accidents, as accidents frequently occur for more than one reason. A difficulty exists in that data are rarely available for each conditional distribution separately. Instead, data are generally available for the overall mixture of distributions and thus the individual contribution by each conditional distribution can not easily be ascertained. Moreover, the potential contributing factors for vehicle accidents are numerous and diverse. Developing a mixture that allows for the separate effect of each potentiality on the overall accident rate would lead to an extremely complex model of little practical use. Instead, it was decided to consider broad categories of factors, and allow each category to have a separate effect on the overall accident rate.

Potential contributing factors are commonly considered to fall into three categories:

1. driver factors (that is, psychological and physiological factors);
2. vehicle factors (such as visibility, lighting, and braking factors); and
3. environmental factors (such as road alignment, weather, and traffic flow factors).

For this study, however, it was decided to not distinguish between the second and third categories, and to consider a model mixing two Poisson densities. It is clear from (2.6) that the theoretical dispersion index must also be greater than or equal to one.

The geometric density is the fourth and final model considered. This density represents, perhaps, an extreme model choice that in practice would be infrequently entertained. The geometric distribution, a special case of the negative binomial distribution, is often referred to as a discrete waiting time distribution, in that it represents how long (in terms of the number of vehicle passages) one has to

wait for an accident to occur. Given the relationship between the geometric and negative binomial distributions, it is evident that this distribution must also have a theoretical dispersion index that ranges on the $(1, \infty)$ interval. Equation (2.8) confirms this property.

From this specification of candidate models, it is apparent that certain nested and nonnested relationships exist between these models. A model is nested within another if the former is a special case of the latter. For example, suppose that M_1 is geometric, with density $f_1(x \mid p) = p\,(1-p)^x$, and M_2 is negative binomial, with density function defined by $f_2(x \mid a, p) = \binom{a+x-1}{x} p^a (1-p)^x$; then it is easy to see then M_1 is nested within M_2 in the sense that we can write $f_1(x \mid p) = f_2(x \mid a = 1, p)$. Nonnested models have no such relationship. Of the candidate models considered here, M_1 is nested within M_3, while M_4 is nested within M_2, so that model discrimination must be made between combinations of nested and nonnested models.

These four models can represent very different interpretations of accidents and could result in quite different inferences if adopted.

2.2 Noninformative prior derivations

A widely used method for determining noninformative priors in a general setting is that of Jeffreys (Berger, 1985). For a distributional function $f_i(\boldsymbol{x} \mid \boldsymbol{\theta}_i)$, where $\boldsymbol{\theta}_i = (\theta_{i1}, \ldots, \theta_{ih})$ is the vector of unknown parameters, this noninformative prior results upon

$$\pi_i^N(\boldsymbol{\theta}_i) = [\det \mathrm{I}(\boldsymbol{\theta}_i)]^{\frac{1}{2}} \tag{2.9}$$

where $\mathrm{I}(\boldsymbol{\theta}_i)$ is the $(h \times h)$ expected Fisher information matrix and 'det' represents the determinant. Under commonly satisfied assumptions this information matrix has element (j, k) equal to

$$\mathrm{I}_{jk}(\boldsymbol{\theta}_i) = -\mathrm{E}_{\boldsymbol{\theta}_i}\left[\frac{\partial^2}{\partial\theta_{ij}\partial\theta_{ik}} \log f_i(\boldsymbol{X} \mid \boldsymbol{\theta}_i)\right].$$

2.2.1 M_1: Poisson

Adopting this strategy, it is easy to derive the Jeffreys noninformative prior for the Poisson density (M_1), which is given by

$$\pi_1^N(\boldsymbol{\theta}_1) = \frac{1}{\sqrt{\lambda}}.$$

In Section 3.4 we demonstrate that this improper noninformative prior yields a proper marginal distribution for all $x_i \geq 0$. This, in turn, implies that a noninformative prior of this form gives a proper posterior for any such x_i.

2.2.2 M_2: Poisson/gamma

Finding a suitable noninformative prior for the Poisson/gamma density (M_2) is somewhat more difficult. However, if the parameters of $\pi_2^N(\boldsymbol{\theta}_2)$ are taken as independent, so that $\pi_2^N(\boldsymbol{\theta}_2) = h_{2,1}(a)\, h_{2,2}(p)$, and recalling that $0 < p < 1$, then a natural noninformative prior distributes p uniformly over the [0,1] interval so that

$$h_{2,2}(p) = \mathcal{U}(0,1).$$

If $h_{2,1}(a)$ is now obtained using the method of Jeffreys then

$$\frac{\partial^2}{\partial a^2} \log f_2(x_i \mid a, p) = \psi'(x_i + a) - \psi'(a)$$

where $\psi(z) = \partial/\partial z \log \Gamma(z)$ and $\psi'(z) = \partial^2/\partial z^2 \log \Gamma(z)$ represent the digamma and trigamma functions, respectively. Asymptotically, as $z \to \infty$, $\psi'(z)$ can be approximated by $1/z$ (equation 6.4.12 of Abramowitz and Stegun, 1965), so that

$$\begin{aligned} \frac{\partial^2}{\partial a^2} \log f_2(x_i \mid a, p) &\approx \frac{1}{x_i + a} - \frac{1}{a} \\ &= \frac{-x_i}{a(x_i + a)}. \end{aligned}$$

Now the approximated expected Fisher information can be given by

$$\begin{aligned} \mathrm{I}(a) &\approx \mathrm{E}_a \left[\frac{X_i}{a(X_i + a)} \right] \\ &= \sum_{x=0}^{\infty} \frac{x_i}{a(x_i + a)} \binom{x_i + a - 1}{x_i} p^a (1-p)^{x_i} \end{aligned}$$

which, when expanded, equals

$$\frac{p^a(1-p)}{(a+1)}\left[1+\frac{(a+1)}{1!}(1-p)\frac{(a+1)}{(a+2)}+\frac{(a+2)(a+1)}{2!}(1-p)^2\frac{(a+1)}{(a+3)}+\ldots\right].$$

Observe that under the same asymptotic conditions, the bracketed term can be approximated by the binomial expansion $(1-(1-p))^{-(a+1)}$ so that

$$\begin{aligned} \mathrm{I}(a) &\approx \frac{p^a(1-p)}{(a+1)}(1-(1-p))^{-(a+1)} \\ &\propto \frac{1}{(a+1)}. \end{aligned}$$

The approximated Jeffreys noninformative prior for $h_{2,1}(a)$ is then

$$h_{2,1}(a) = \frac{1}{\sqrt{a+1}}$$

and so an appropriate noninformative prior for the Poisson/gamma density is given by

$$\pi_2^N(\boldsymbol{\theta}_2) = \frac{1}{\sqrt{a+1}}.$$

Again, in Section 3.4 we demonstrate that a noninformative prior of this form ensures a proper marginal distribution, and hence a proper posterior distribution, for all $x_i \geq 0$.

It could be suggested that a simple noninformative choice for $h_{2,1}(a)$ would be $h_{2,1}(a) \equiv 1$. However, when $h_{2,1}(a) \equiv 1$ is applied, the resultant posterior distribution is never proper for any x_i. Should $h_{2,2}(p)$ be derived using the method of Jeffreys, then $h_{2,2}(p) \propto 1/p\sqrt{1-p}$. It is easy to verify that a prior of this form, used in conjunction with the Jeffreys noninformative prior for $h_{2,1}(a)$, does not give a proper posterior density for $x_i = 0$. Additionally, the "joint" Jeffreys prior derived directly from (2.9) is complicated and of little practical use.

2.2.3 M_3: mixture of two Poissons

A noninformative prior for the mixture of two Poisson densities (M_3) is difficult to derive from the approach of Jeffreys, as M_3 is not from an exponential family. If the parameters $\{p\}$ and $\{\lambda_1, \lambda_2\}$ of $\pi_3^N(\boldsymbol{\theta}_3)$ are treated as independent, so that $\pi_3^N(\boldsymbol{\theta}_3) = h_{3,1}(p)h_{3,\cdot}(\lambda_1, \lambda_2)$, and assuming the conditional relationship $h_{3,\cdot}(\lambda_1, \lambda_2) =$

$h_{3,2}(\lambda_1 \mid \lambda_2)\, h_{3,3}(\lambda_2)$, then an appropriate noninformative prior can be constructed using the following rationale.

As before, a natural noninformative prior for p is uniform support over the $[0, 1]$ interval so that $h_{3,1}(p) = \mathcal{U}(0, 1)$. Now, λ_2 is a rate parameter from a Poisson distribution so, as seen in M_1, a sensible noninformative specification for this parameter is $h_{3,3}(\lambda_2) = 1/\sqrt{\lambda_2}$. Lastly, conditional upon λ_2 and noting that $0 < \lambda_1 < \lambda_2$, a natural noninformative prior distributes λ_1 uniformly over the $[0, \lambda_2]$ interval, so that $h_{3,2}(\lambda_1 \mid \lambda_2) = 1/\lambda_2$. When combined, this yields

$$\begin{aligned} \pi_3^N(\boldsymbol{\theta}_3) &= h_{3,1}(p)\, h_{3,2}(\lambda_1 \mid \lambda_2)\, h_{3,3}(\lambda_2) \\ &= \frac{1}{\lambda_2^{3/2}} \end{aligned}$$

which results in a proper marginal (see Section 3.4) and hence a proper posterior distribution for all $x_i \geq 0$.

It could be suggested that a simple noninformative choice for $h_{3,2}(\lambda_1 \mid \lambda_2)$ would be $h_{3,2}(\lambda_1 \mid \lambda_2) \equiv 1$, leading to $\pi_3^N(\boldsymbol{\theta}_3) = 1/\sqrt{\lambda_2}$. However, if applied, it is easy to verify that this noninformative prior results in a posterior distribution that is not defined for any x_i.

2.2.4 M_4: geometric

Finally, the noninformative prior for the geometric distribution (M_4) using the method of Jeffreys can easily be ascertained as

$$\pi_4^N(\boldsymbol{\theta}_4) = \frac{1}{p\sqrt{1-p}}$$

which results in a proper marginal (see Section 3.4) and hence a proper posterior distribution for all $x_i \geq 0$.

Chapter 3

Model Discrimination

3.1 Preliminaries

3.1.1 Bayes factors

Bayes factors have long been employed to discriminate between competing models; see Kass and Raftery (1995) for a good review and list of references.

A Bayes factor can be derived as follows: suppose it is believed *a priori* that any of κ statistical models $M_1, \ldots, M_\kappa$ could be used to describe a vector of data $\boldsymbol{x} = (x_1, \ldots, x_n)$; each model having some density $f_i(\boldsymbol{x} \mid \boldsymbol{\theta}_i)$. The parameter vector $\boldsymbol{\theta}_i$ is unknown and has dimension h_i for $i = 1, \ldots, \kappa$ respectively. Should $\pi_i(\boldsymbol{\theta}_i)$ represent the elicited prior distribution of the parameters for M_i then the Bayes factor comparing M_j to M_i, denoted by B_{ji}, is given by

$$B_{ji} = \frac{m_j(\boldsymbol{x})}{m_i(\boldsymbol{x})} = \frac{\int f_j(\boldsymbol{x} \mid \boldsymbol{\theta}_j)\, \pi_j(\boldsymbol{\theta}_j)\, d\boldsymbol{\theta}_j}{\int f_i(\boldsymbol{x} \mid \boldsymbol{\theta}_i)\, \pi_i(\boldsymbol{\theta}_i)\, d\boldsymbol{\theta}_i} \tag{3.1}$$

where $m_i(\boldsymbol{x})$ is the marginal or predictive distribution of $\boldsymbol{X}$ under model M_i. Bayes factors thus summarise the evidence provided by the data in favour of one statistical model compared to its competitor.

Kass and Raftery (1995) recommend the guide-lines included in Table 3.1 for interpreting B_{ji}.

Table 3.1: Guide-lines for interpreting B_{ji}.

B_{ji}	Evidence for M_i	B_{ji}	Evidence for M_j
$< 1/150$	Very Strong	1 to 3	Minimal
1/150 to 1/20	Strong	3 to 20	Positive
1/20 to 1/3	Positive	20 to 150	Strong
1/3 to 1	Minimal	> 150	Very Strong

Clearly (3.1) implies what Berger and Pericchi (1996) call *multiple model coherency*; that is

$$B_{ji} = \frac{1}{B_{ij}} \quad \text{and similarly} \quad B_{ji} = \frac{B_{jk}}{B_{ik}} \tag{3.2}$$

for M_i, M_j and M_k comparisons. Should $p(M_i)$ describe the prior probability assertion for model M_i, then using the appropriate pairwise Bayes factor comparisons, the posterior probability for this model is given by

$$P(M_i \mid \boldsymbol{x}) = \left(\sum_{j=1}^{\kappa} \frac{p(M_j)}{p(M_i)} B_{ji} \right)^{-1}. \tag{3.3}$$

The desirable *multiple model coherency* property of (3.2) ensures that order has no bearing on the resultant support for any candidate model, that model support is consistent across comparisons and that posterior probabilities, as defined in (3.3), sum (over all κ models) to unity.

Difficulty arises in the need to specify prior distributions, $\pi_i(\boldsymbol{\theta}_i)$, for each model entertained. In some circumstances, careful subjective elicitation and specification of these prior distributions is not feasible. The inability to formulate informative prior densities may result when the practitioner has little intuition or familiarity with the collection of candidate models under investigation and time or money constraints do not allow elicitation from other sources. Alternatively, it may result from the lack of suitable quality information to specify appropriate prior distributions. In such cases, noninformative priors should be adopted.

A noninformative prior is a prior which contains no information about the unknown parameters of interest (namely the vector $\boldsymbol{\theta}_i$ for model M_i). More crudely,

it is a prior which "favours" no possible value of $\boldsymbol{\theta}_i$ over any others. Even with the availability of informative prior information, noninformative priors are often employed to offer an *automated* or *objective* Bayesian analysis.

Noninformative priors (denoted by $\pi_i^N(\boldsymbol{\theta}_i)$) are frequently improper, in that they have infinite mass, and are typically written as

$$\pi_i^N(\boldsymbol{\theta}_i) \propto h_i(\boldsymbol{\theta}_i)$$

where $h_i(\boldsymbol{\theta}_i)$ is some function on $\boldsymbol{\theta}_i$. For example, the uniform prior is often expressed as $\pi_i^N(\boldsymbol{\theta}_i) \propto 1$.

Formally, we can write

$$\pi_i^N(\boldsymbol{\theta}_i) = c_i\, h_i(\boldsymbol{\theta}_i)$$

where c_i is treated as some unspecified normalising constant. Ensuing Bayesian analysis involving a single model results in a posterior distribution for the unknown parameter $\boldsymbol{\theta}_i$ of the form

$$\begin{aligned} \pi_i(\boldsymbol{\theta}_i \mid \boldsymbol{x}) &= \frac{f_i(\boldsymbol{x} \mid \boldsymbol{\theta}_i)\, \pi_i^N(\boldsymbol{\theta}_i)}{\int f_i(\boldsymbol{x} \mid \boldsymbol{\theta}_i)\, \pi_i^N(\boldsymbol{\theta}_i)\, d\boldsymbol{\theta}_i} \\ &= \frac{c_i\, f_i(\boldsymbol{x} \mid \boldsymbol{\theta}_i)\, h_i(\boldsymbol{\theta}_i)}{c_i \int f_i(\boldsymbol{x} \mid \boldsymbol{\theta}_i)\, h_i(\boldsymbol{\theta}_i)\, d\boldsymbol{\theta}_i}. \end{aligned} \tag{3.4}$$

Notice that the unspecified normalising constants c_i in (3.4) cancel out. Elimination of these constants implies that if $\int f_i(\boldsymbol{x} \mid \boldsymbol{\theta}_i)\, h_i(\boldsymbol{\theta}_i)\, d\boldsymbol{\theta}_i$ is proper (i.e. has finite mass) then the posterior density (3.4) is also proper, despite c_i being unspecified.

When dealing with more than a single model, as in (3.1), the resultant Bayes factors are typically defined up to

$$B_{ji}^N = \frac{m_j^N(\boldsymbol{x})}{m_i^N(\boldsymbol{x})} = \frac{c_j \int f_j(\boldsymbol{x} \mid \boldsymbol{\theta}_j)\, h_j(\boldsymbol{\theta}_j)\, d\boldsymbol{\theta}_j}{c_i \int f_i(\boldsymbol{x} \mid \boldsymbol{\theta}_i)\, h_i(\boldsymbol{\theta}_i)\, d\boldsymbol{\theta}_i} \tag{3.5}$$

where $m_i^N(\boldsymbol{x}) = \int f_i(\boldsymbol{x} \mid \boldsymbol{\theta}_i)\, \pi_i^N(\boldsymbol{\theta}_i)\, d\boldsymbol{\theta}_i$ is the marginal distribution for model i based on a noninformative prior. Equation (3.5) depends on the unspecified c_j/c_i ratio and hence is unsatisfactory for selection purposes.

Various attempts at addressing and eliminating this unspecified c_j/c_i ratio inherent within (3.5) have been propounded, including several techniques using training samples and partial likelihood methods. These training samples and partial likelihood methods have considerable appeal and form the basis for the derivation of the averaged Bayes factor.

3.1.2 Training samples and partial likelihood methods

It may be possible to use a part of the data within a given model to compute a proper posterior distribution using a noninformative prior. This proper posterior can then be adopted as a *prior* density so that Bayes factors can be derived from the remaining data. A sample used for the development of the prior posterior distribution is called a *training sample*. Thus a training sample is a special subset of the given data that allows the specification of a proper posterior distribution free from unspecified normalising constant multipliers. Such posteriors used as prior distributions ensure that subsequent Bayes factor derivations can be usefully employed for discrimination purposes, despite the absence of prior information.

Suppose that $\boldsymbol{x}(l)$ is some subset of the data and $\boldsymbol{x}(l')$ denotes those observed data outside this subset, so that $\boldsymbol{x} = \{\boldsymbol{x}(l), \boldsymbol{x}(l')\} = (x_1, \ldots, x_n)$. For example, $\boldsymbol{x}(l) = \{x_1, \ldots, x_i\}$ and $\boldsymbol{x}(l') = \{x_{i+1}, \ldots, x_n\}$ represents one such partition of the n data points. Now $\boldsymbol{x}(l)$, the training sample, can be used to convert the improper noninformative prior $\pi_i^N(\boldsymbol{\theta}_i)$ to a proper posterior $\pi_i^N(\boldsymbol{\theta}_i \mid \boldsymbol{x}(l))$ for model M_i, by noting

$$\begin{aligned} \pi_i^N(\boldsymbol{\theta}_i \mid \boldsymbol{x}(l)) &= \frac{f_i(\boldsymbol{x}(l) \mid \boldsymbol{\theta}_i)\, \pi_i^N(\boldsymbol{\theta}_i)}{m_i^N(\boldsymbol{x}(l))} \\ &= \frac{c_i\, f_i(\boldsymbol{x}(l) \mid \boldsymbol{\theta}_i)\, h_i(\boldsymbol{\theta}_i)}{c_i \int f_i(\boldsymbol{x}(l) \mid \boldsymbol{\theta}_i)\, h_i(\boldsymbol{\theta}_i)\, d\boldsymbol{\theta}_i} \end{aligned} \tag{3.6}$$

where, again, c_i is an unspecified normalising constant and

$$m_i^N(\boldsymbol{x}(l)) = \int f_i(\boldsymbol{x}(l) \mid \boldsymbol{\theta}_i)\, \pi_i^N(\boldsymbol{\theta}_i)\, d\boldsymbol{\theta}_i \tag{3.7}$$

is the marginal density of the training sample under M_i. Observe that c_i cancels out in (3.6). Using the remainder of the data, denoted by $\boldsymbol{x}(l')$, the Bayes factor is given by

$$B_{ji}^N(l) = \frac{\int f_j(\boldsymbol{x}(l') \mid \boldsymbol{\theta}_j, \boldsymbol{x}(l))\, \pi_j^N(\boldsymbol{\theta}_j \mid \boldsymbol{x}(l))\, d\boldsymbol{\theta}_j}{\int f_i(\boldsymbol{x}(l') \mid \boldsymbol{\theta}_i, \boldsymbol{x}(l))\, \pi_i^N(\boldsymbol{\theta}_i \mid \boldsymbol{x}(l))\, d\boldsymbol{\theta}_i} \tag{3.8}$$

which is free from the unwanted ratio of unspecified normalising constants, as desired.

Training samples should be large enough so that $\pi_i^N(\boldsymbol{\theta}_i \mid \boldsymbol{x}(l))$ is proper for all candidate models (that is $0 < \pi_i^N(\boldsymbol{\theta}_i \mid \boldsymbol{x}(l)) < \infty$ for $i = 1, \ldots, \kappa$) yet they should

be as small as possible so that most of the data can be used in calculations for the weighted likelihood ratio of models M_j to M_i in (3.8). For $\pi_i^N(\boldsymbol{\theta}_i \mid \boldsymbol{x}(l))$ to be proper for all κ candidate models, then $m_i^N(\boldsymbol{x}(l))$, $i = 1, \ldots \kappa$, given by (3.7) must also be proper. These notions are formalised by the following definition given by Berger and Pericchi (1996).

Definition. A training sample, $\boldsymbol{x}(l)$, is called *proper* if $0 < m_i^N(\boldsymbol{x}(l)) < \infty$ for all M_i, and *minimal* if it is proper and no subset is proper.

Typically, for a particular data set $\boldsymbol{x}$, there are many varied minimal training sample partitions. The Bayes factor defined by (3.8) is clearly dependent on the particular minimal training sample selected and hence adoption of different training samples will result in different Bayes factors. It is this fact that we now exploit with the introduction of the *averaged Bayes factor*.

3.2 Averaged Bayes factor

The Bayes factor $B_{ji}^N(l)$ defined in (3.8) depends on the particular minimal training sample chosen. To eliminate this dependency, and increase stability, the averaged Bayes factor is introduced as follows.

Let $\mathcal{X}_T = \{\boldsymbol{x}(1), \boldsymbol{x}(2), \ldots, \boldsymbol{x}(L)\}$ denote the set of all minimal training samples, $\boldsymbol{x}(l)$. The principle idea is to take an average of the posterior densities $\pi_i^N(\boldsymbol{\theta}_i \mid \boldsymbol{x}(l))$, given in (3.6), over all L combinations of minimal training samples $\boldsymbol{x}(l) \in \mathcal{X}_T$ for each model under investigation. Associated averaged distributions are subsequently used as the prior distribution in (3.1), so that a pseudo-marginal distribution can be ascertained for each respective model under comparison. Derivation of the averaged Bayes factor naturally ensues with the pairwise comparisons of these pseudo-marginal distributions.

Mathematically, we define the pseudo-marginal distribution of $\boldsymbol{X}$ under model M_i as

$$\overline{m}_i^N(\boldsymbol{x}) = \int f_i(\boldsymbol{x} \mid \boldsymbol{\theta}_i) \frac{1}{L} \sum_{l=1}^{L} \pi_i^N(\boldsymbol{\theta}_i \mid \boldsymbol{x}(l))\, d\boldsymbol{\theta}_i \tag{3.9}$$

thus the averaged Bayes factor, B_{ji}^{A}, for model comparison M_j to M_i, is given by

$$B_{ji}^{A} = \frac{\overline{m}_j^N(\boldsymbol{x})}{\overline{m}_i^N(\boldsymbol{x})}. \tag{3.10}$$

From this derivation of the averaged Bayes factor it is clear that the following properties hold.

Properties

1. The formulation of the averaged Bayes factor ensures that the ratio of unspecified constants in (3.5) is eliminated.

2. The pseudo-marginal distribution $\overline{m}_i^N(\boldsymbol{x})$, given by (3.9), can be independently computed for each of the κ candidate models. This is important and computationally advantageous, because once $\overline{m}_i^N(\boldsymbol{x})$ is numerically ascertained *any* pairwise comparison involving M_i can then be conducted. Some averaging techniques do not enjoy this property.

3. The important multiple model coherency property of (3.2) is preserved. This is due to (3.10) being composed from the ratio of independently computed $\overline{m}_i^N(\boldsymbol{x})$ distributions for pairwise model comparisons.

4. The averaged Bayes factor is a fully automated criterion, in that it only requires standard noninformative priors for its computation. Moreover, due to the averaging process in (3.9), it is relatively insensitive to the particular noninformative prior density used, so that reference priors, Jeffreys priors or other appropriately derived noninformative priors can be adopted without substantially affecting the resultant Bayes factor. Not all noninformative Bayes factor methods are able to make this assurance.

5. Selection using (3.10) can be made for nested or nonnested models, and for multiple model comparisons.

6. Stability of resultant factors and independence from particular training data is assured by the averaging of $\pi_i^N(\boldsymbol{\theta}_i \mid \boldsymbol{x}(l))$ over all L minimal training samples $\boldsymbol{x}(l) \in \mathcal{X}_T$. This is because any unusual training sample will contribute only a small fraction (in fact $1/L$) of the prior information used for the derivation of the marginal density $\overline{m}_i^N(\boldsymbol{x})$.

This averaged Bayes factor method, therefore, appears to have some distinct advantages over current noninformative variants of the Bayes factor.

To contrast the averaged Bayes factor, we use the most commonly adopted Bayesian discrimination method, the *Bayesian information criterion*. This approach is the topic of the next section.

3.3 Bayesian information criterion

The most conventionally employed "Bayesian" model selection technique is that of the renowned Bayesian information criterion (BIC) introduced by Schwarz (1978). For conditionally independent data this criterion has been modified by various authors (such as Raftery, 1993, and Raftery, 1995) so that the Bayes factor given in (3.1) can be approximated by

$$B_{ji}^{S} = \frac{f_j(\boldsymbol{x} \mid \widehat{\boldsymbol{\theta}}_j)}{f_i(\boldsymbol{x} \mid \widehat{\boldsymbol{\theta}}_i)} \, n^{-(h_j - h_i)/2} \tag{3.11}$$

where $\widehat{\boldsymbol{\theta}}_i$ is the vector of maximum likelihood estimates (MLE) under M_i and, as before, h_i is the dimension of the parameter vector $\boldsymbol{\theta}_i$. The model selection criterion (3.11) is typically reported as $2\log_e B_{ji}^{S}$, which has parallels with the standard likelihood ratio test statistic for testing M_i against M_j (Raftery, 1995).

The asymptotic principles and simplifications used to derive the BIC criterion and its approximations are satisfactory when dealing with large samples. Subsequent examination has revealed that serious biases can manifest themselves when these criteria are applied to samples of small size (O'Hagan, 1995, Berger and Pericchi, 1996). Indeed, the asymptotically constant term that is ignored in the development of (3.11) can dominate the Bayes factor under such circumstances. As this term can be either arbitrarily large or small, the BIC criterion can systematically bias the results in favour of either the simpler or the more complicated model under comparison. Moreover, this bias can be quite substantial.

Accident data are generally available at individual sites for a small number of years. This suggests that the BIC criterion, and other methods based upon similar asymptotic principles and approximations, may contain serious systematic bias, rendering them unsuitable for model selection purposes in much of the accident analysis framework.

The BIC criterion is further hampered by the fact that informative prior information pertaining to the unknown parameters of interest cannot be embodied within the model, something that *strictly* Bayesian methods should facilitate.

3.4 Numerical example

Model discrimination between the four candidate models introduced in Section 2.1 is now undertaken. Discrimination is conducted separately at each of the 35 traffic accident intersection sites included in Table A.1 of Appendix A and at the hypothetical Site B. In all instances it is assumed that insufficient resources are available to construct informative prior densities, necessitating the embodiment of noninformative priors. For convenience, those noninformative priors delineated within Section 2.2 will be employed.

Discrimination is initially conducted using the averaged Bayes factor and then, for comparison, this discrimination is repeated using the approximated BIC method.

3.4.1 Averaged Bayes factor

The derivation of the marginal distributions, as defined in (3.7), based upon a training sample of just a single observation, $\boldsymbol{x}(l) = \{x_j\}$, is easily undertaken for the four candidate models.

Marginal distribution: $m_1^N(\boldsymbol{x}(l))$

Recall from (3.7) that

$$m_i^N(\boldsymbol{x}(l)) = \int f_i(\boldsymbol{x}(l) \mid \boldsymbol{\theta}_i)\, \pi_i^N(\boldsymbol{\theta}_i)\, d\boldsymbol{\theta}_i$$

then for M_1, the Poisson distribution,

$$\begin{aligned} m_1^N(\boldsymbol{x}(l)) &= \int_0^\infty \frac{\lambda^{x_j} e^{-\lambda}}{x_j!} \frac{1}{\sqrt{\lambda}} d\lambda \\ &= \frac{1}{x_j!} \int_0^\infty \lambda^{x_j - 1/2} e^{-\lambda} d\lambda \end{aligned}$$

and recognising the form of the gamma distribution, providing $x_j + 1/2 > 0$, then

$$\begin{aligned} m_1^N(\boldsymbol{x}(l)) &= \frac{\Gamma(x_j+1/2)}{x_j!}\int_0^\infty \frac{\lambda^{(x_j+1/2)-1}e^{-\lambda}}{\Gamma(x_j+1/2)}d\lambda \\ &= \frac{\Gamma(x_j+1/2)}{\Gamma(x_j+1)} \end{aligned}$$

which is proper for all $x_j \geq 0$.

Marginal distribution: $m_2^N(\boldsymbol{x}(l))$

For M_2, the Poisson/gamma density, the marginal is defined by

$$m_2^N(\boldsymbol{x}(l)) = \int_0^1 \int_0^\infty \binom{x_j+a-1}{x_j} p^a(1-p)^{x_j}\frac{1}{\sqrt{a+1}}\,da\,dp.$$

Recognising the form of the beta distribution, providing $a+1>0$ and $x_j+1>0$, hence integrating with respect to p and then with respect to a gives

$$\begin{aligned} m_2^N(\boldsymbol{x}(l)) &= \int_0^\infty \binom{x_j+a-1}{x_j}\frac{1}{\sqrt{a+1}}\frac{\Gamma(a+1)\,\Gamma(x_j+1)}{\Gamma(x_j+a+2)} \times \\ &\quad \int_0^1 \frac{\Gamma(x_j+a+2)}{\Gamma(a+1)\,\Gamma(x_j+1)}p^{(a+1)-1}(1-p)^{(x_j+1)-1}dp\,da \\ &= \int_0^\infty \frac{a}{(x_j+a)\,(x_j+a+1)\,\sqrt{a+1}}\,da \\ &= \begin{cases} 2 & \text{for } x_j = 0 \\ \pi - 2 & \text{for } x_j = 1 \\ x_j\left[2\arctan(1/\sqrt{x_j-1}) - \pi\right]/\sqrt{x_j-1} \;+ & \\ (x_j+1)\left[\pi - 2\arctan(1/\sqrt{x_j})\right]/\sqrt{x_j} & \text{for } x_j \geq 2, \end{cases} \end{aligned} \tag{3.12}$$

which is proper for all $x_j \geq 0$.

Marginal distribution: $m_3^N(\boldsymbol{x}(l))$

For M_3, the mixture of two Poisson densities,

$$m_3^N(\boldsymbol{x}(l)) = \int\int\int \left[p\frac{\lambda_1^{x_j}e^{-\lambda_1}}{x_j!} + (1-p)\frac{\lambda_2^{x_j}e^{-\lambda_2}}{x_j!}\right]\frac{1}{\lambda_2^{3/2}}\,dp\,d\lambda_1\,d\lambda_2$$

$$= \int\int\int p \frac{\lambda_1^{x_j} e^{-\lambda_1}}{x_j!} \frac{1}{\lambda_2^{3/2}}\, dp\, d\lambda_1\, d\lambda_2 + \qquad \text{(term 1)}$$

$$\int\int\int (1-p) \frac{\lambda_2^{x_j} e^{-\lambda_2}}{x_j!} \frac{1}{\lambda_2^{3/2}}\, dp\, d\lambda_1\, d\lambda_2 \qquad \text{(term 2)}.$$

Consider initially term 1. Integrating with respect to p and then with respect to λ_2 (recalling that $0 < \lambda_1 < \lambda_2 < \infty$) gives

$$\int_0^\infty \int_{\lambda_1}^\infty \frac{\lambda_1^{x_j} e^{-\lambda_1}}{x_j!} \frac{1}{\lambda_2^{3/2}} \int_0^1 p\, dp\, d\lambda_2\, d\lambda_1 = \frac{1}{2} \int_0^\infty \frac{\lambda_1^{x_j} e^{-\lambda_1}}{x_j!} \int_{\lambda_1}^\infty \frac{1}{\lambda_2^{3/2}}\, d\lambda_2\, d\lambda_1$$

$$= \int_0^\infty \frac{\lambda_1^{x_j - 1/2} e^{-\lambda_1}}{x_j!}\, d\lambda_1.$$

Recognising the form of the gamma distribution, providing $x_j + 1/2 > 0$, then

$$\int_0^\infty \frac{\lambda_1^{x_j - 1/2} e^{-\lambda_1}}{x_j!}\, d\lambda_1 = \frac{\Gamma(x_j + 1/2)}{x_j!} \int_0^\infty \frac{\lambda_1^{(x_j + 1/2) - 1} e^{-\lambda_1}}{\Gamma(x_j + 1/2)}\, d\lambda_1$$

$$= \frac{\Gamma(x_j + 1/2)}{\Gamma(x_j + 1)}$$

which is proper for all $x_j \geq 0$. Now consider term 2. Integrating with respect to p and then λ_1 gives

$$\int_0^\infty \int_0^{\lambda_2} \frac{\lambda_2^{x_j - 3/2} e^{-\lambda_2}}{x_j!} \int_0^1 (1-p)\, dp\, d\lambda_1\, d\lambda_2 = \frac{1}{2} \int_0^\infty \frac{\lambda_2^{x_j - 3/2} e^{-\lambda_2}}{x_j!} \int_0^{\lambda_2} 1\, d\lambda_1\, d\lambda_2$$

$$= \frac{1}{2} \int_0^\infty \frac{\lambda_2^{x_j - 1/2} e^{-\lambda_2}}{x_j!}\, d\lambda_2.$$

Again recognising the form of the gamma distribution, providing $x_j + 1/2 > 0$, then

$$\frac{1}{2} \int_0^\infty \frac{\lambda_2^{x_j - 1/2} e^{-\lambda_2}}{x_j!}\, d\lambda_2 = \frac{\Gamma(x_j + 1/2)}{2 x_j!} \int_0^\infty \frac{\lambda_2^{(x_j + 1/2) - 1} e^{-\lambda_2}}{\Gamma(x_j + 1/2)}\, d\lambda_2$$

$$= \frac{\Gamma(x_j + 1/2)}{2\,\Gamma(x_j + 1)}$$

which is also proper for all $x_j \geq 0$. Combining both terms 1 and 2 yields,

$$m_3^N(\boldsymbol{x}(l)) = \frac{3\,\Gamma(x_j + 1/2)}{2\,\Gamma(x_j + 1)}.$$

Marginal distribution: $m_4^N(\boldsymbol{x}(l))$

Lastly, for M_4, the geometric density,

$$\begin{aligned} m_4^N(\boldsymbol{x}(l)) &= \int_0^1 p(1-p)^{x_j} \frac{1}{p\sqrt{1-p}}\, dp \\ &= \int_0^1 (1-p)^{x_j - 1/2}\, dp \\ &= \frac{1}{x_j + 1/2} \end{aligned}$$

which is proper for all $x_j \geq 0$.

Minimal training sample

A minimal training sample thus consists of a single observation, $\boldsymbol{x}(l) = \{x_j\}$, provided that $x_j \geq 0$. This condition on x_j is clearly satisfied for our accident data.

For this numerical example it is also apparent that $\mathcal{X}_T$, the set of all minimal training samples, has n members so that $L = n$.

Pseudo-marginal distribution: $\overline{m}_1^N(\boldsymbol{x})$

The pseudo-marginal distribution $\overline{m}_1^N(\boldsymbol{x})$, as defined in (3.9), can be expressed in closed form. Its derivation can be found using the following rationale.

$$\begin{aligned} \overline{m}_1^N(\boldsymbol{x}) &= \int f_1(\boldsymbol{x} \mid \boldsymbol{\theta}_1) \left[\frac{1}{L} \sum_{l=1}^{L} \pi_1^N(\boldsymbol{\theta}_1 \mid \boldsymbol{x}(l)) \right] d\boldsymbol{\theta}_1 \\ &= \frac{1}{n} \int f_1(\boldsymbol{x} \mid \boldsymbol{\theta}_1)\, \pi_1^N(\boldsymbol{\theta}_1 \mid \boldsymbol{x}(1))\, d\boldsymbol{\theta}_1 + \ldots + \frac{1}{n} \int f_1(\boldsymbol{x} \mid \boldsymbol{\theta}_1)\, \pi_1^N(\boldsymbol{\theta}_1 \mid \boldsymbol{x}(n))\, d\boldsymbol{\theta}_1 \end{aligned}$$

after expanding the summation and noting $L = n$. Now considering the jth term, then

$$\begin{aligned} \pi_1^N(\boldsymbol{\theta}_1 \mid \boldsymbol{x}(j)) &= \frac{f_1(\boldsymbol{x}(j) \mid \boldsymbol{\theta}_1)\, \pi_1(\boldsymbol{\theta}_1)}{\int f_1(\boldsymbol{x}(j) \mid \boldsymbol{\theta}_1)\, \pi_1(\boldsymbol{\theta}_1)\, d\boldsymbol{\theta}_1} \\ &= \frac{f_1(x_j \mid \boldsymbol{\theta}_1)\, \pi_1(\boldsymbol{\theta}_1)}{m_1^N(\boldsymbol{x}(j))} \\ &= \frac{\lambda^{x_j - 1/2} e^{-\lambda}}{\Gamma(x_j + 1/2)} \end{aligned}$$

which is clearly recognisable as having the form of a gamma density. Under the aforementioned assumption of conditionally independent data, which implies

$$f_k(\boldsymbol{x} \mid \boldsymbol{\theta}_k) = \prod_{i=1}^{n} f_k(x_i \mid \boldsymbol{\theta}_k)$$

for any given M_k, then

$$\begin{aligned} \int f_1(\boldsymbol{x} \mid \boldsymbol{\theta}_1)\, \pi_1^N(\boldsymbol{\theta}_1 \mid \boldsymbol{x}(j))\, d\boldsymbol{\theta}_1 &= \int_0^\infty \left[\prod_{i=1}^{n} \frac{\lambda^{x_i} e^{-\lambda}}{x_i!}\right] \frac{\lambda^{x_j - 1/2} e^{-\lambda}}{\Gamma(x_j + 1/2)}\, d\lambda \\ &= \left[\prod_{i=1}^{n} \frac{1}{x_i!}\right] \frac{1}{\Gamma(x_j + 1/2)} \int_0^\infty \lambda^{S + x_j - 1/2} e^{-(n+1)\lambda}\, d\lambda \end{aligned}$$

where $S = \sum_{i=1}^{n} x_i$. Exploiting the form of the gamma density, providing that $S + x_j + 1/2 > 0$ (which is always true for accident counts), this intergal can be rewritten as

$$\left[\prod_{i=1}^{n} \frac{1}{x_i!}\right] \frac{\Gamma(S + x_j + 1/2)}{\Gamma(x_j + 1/2)\,(n+1)^{S + x_j + 1/2}} \int_0^\infty \frac{(n+1)^{S + x_j + 1/2}}{\Gamma(S + x_j + 1/2)} \lambda^{(S + x_j + 1/2) - 1} e^{-(n+1)\lambda}\, d\lambda$$

which integrates out to

$$\left[\prod_{i=1}^{n} \frac{1}{x_i!}\right] \frac{\Gamma(S + x_j + 1/2)}{\Gamma(x_j + 1/2)\,(n+1)^{S + x_j + 1/2}}.$$

Now, summing over the n terms gives

$$\overline{m}_1^N(\boldsymbol{x}) = \frac{1}{n} \left[\prod_{i=1}^{n} \frac{1}{x_i!}\right] \sum_{j=1}^{n} \frac{\Gamma(S + x_j + 1/2)}{\Gamma(x_j + 1/2)} (n+1)^{-S - x_j - 1/2}.$$

Pseudo-marginal distribution: $\overline{m}_2^N(\boldsymbol{x})$

Numerical integration is necessary for the computation of $\overline{m}_2^N(\boldsymbol{x})$, although only n one-dimensional integrations over a are required as the integration over p can be done in closed form.

The posterior distribution based upon the jth training sample is

$$\pi_2^N(\boldsymbol{\theta}_2 \mid \boldsymbol{x}(j)) = \frac{1}{m_2(\boldsymbol{x}(j))} \binom{x_j + a - 1}{x_j} \frac{p^a (1-p)^{x_j}}{\sqrt{a+1}}$$

where $m_2(\boldsymbol{x}(j))$ is given by (3.12). The jth term of the pseudo-marginal distribution is thus

$$\frac{1}{n}\int f_2(\boldsymbol{x} \mid \boldsymbol{\theta}_2)\,\pi_2^N(\boldsymbol{\theta}_2 \mid \boldsymbol{x}(j))\,d\boldsymbol{\theta}_2$$

$$= \frac{1}{n}\int\int \left[\prod_{i=1}^{n}\binom{x_i+a-1}{x_i} p^a(1-p)^{x_i}\right] \frac{1}{m_2(\boldsymbol{x}(j))}\binom{x_j+a-1}{x_j}\frac{p^a(1-p)^{x_j}}{\sqrt{a+1}}\,da\,dp$$

$$= C\int_0^\infty \left[\prod_{i=1}^{n}\binom{x_i+a-1}{x_i}\right]\frac{1}{\sqrt{a+1}}\binom{x_j+a-1}{x_j}\int_0^1 p^{(n+1)a}(1-p)^{S+x_j}\,dp\,da.$$

where $C = [n\,m_2(\boldsymbol{x}(j))]^{-1}$. Recognising the form of the beta distribution, providing $(n+1)a+1>0$ and $S+x_j+1>0$, this integration equals

$$C\int_0^\infty \left[\prod_{i=1}^{n}\binom{x_i+a-1}{x_i}\right]\binom{x_j+a-1}{x_j}\frac{B(S+x_j+1,(n+1)a+1)}{\sqrt{a+1}}\times$$
$$\int_0^1 \frac{p^{((n+1)a+1)-1}(1-p)^{(S+x_j+1)-1}}{B(S+x_j+1,(n+1)a+1)}dp\,da,$$

where $B(x,y)$ is the beta function with relation $B(x,y) = \Gamma(x)\,\Gamma(y)/\Gamma(x+y)$. Integrating with respect to p yields

$$C\int_0^\infty \left[\prod_{i=1}^{n}\binom{x_i+a-1}{x_i}\right]\binom{x_j+a-1}{x_j}\frac{B(S+x_j+1,(n+1)a+1)}{\sqrt{a+1}}\,da.$$

Lastly, replacing C and summing over the n terms gives

$$\overline{m}_2^N(\boldsymbol{x}) = \frac{1}{n}\sum_{j=1}^{n}\frac{1}{m_2^N(\boldsymbol{x}(j))}\times$$
$$\int_0^\infty \left[\prod_{i=1}^{n}\binom{x_i+a-1}{x_i}\right]\binom{x_j+a-1}{x_j}\frac{B(S+x_j+1,(n+1)a+1)}{\sqrt{a+1}}\,da.$$

Pseudo-marginal distribution: $\overline{m}_3^N(\boldsymbol{x})$

The term $\overline{m}_3^N(\boldsymbol{x})$ can not be readily simplified so the solution must be achieved through three-dimensional numerical integration.

Pseudo-marginal distribution: $\overline{m}_4^N(\boldsymbol{x})$

Using a similar rationale to that used for the derivation of $\overline{m}_1^N(\boldsymbol{x})$, the pseudo-marginal distribution can be written in closed form for M_4. This is done by noting the posterior distribution based upon the jth training sample is

$$\pi_4^N(\boldsymbol{\theta}_4 \mid \boldsymbol{x}(j)) = (x_j+1/2)(1-p)^{x_j-1/2}$$

and so the jth term of the pseudo-marginal is given by

$$\begin{aligned}
&\frac{1}{n}\int f_4(\boldsymbol{x} \mid \boldsymbol{\theta}_4)\, \pi_4^N(\boldsymbol{\theta}_4 \mid \boldsymbol{x}(j))\, d\boldsymbol{\theta}_4 \\
&= \frac{1}{n}\int_0^1 \left[\prod_{i=1}^{n} p(1-p)^{x_i}\right] (x_j + 1/2)(1-p)^{x_j - 1/2} dp \\
&= \frac{(x_j + 1/2)}{n}\int_0^1 p^n (1-p)^{S + x_j - 1/2} dp.
\end{aligned}$$

Recognising the form of the beta density, providing $n+1 > 0$ and $S + x_j + 1/2 > 0$, this integral can be rewritten as

$$\begin{aligned}
&\frac{(x_j + 1/2)}{n} B(S + x_j + 1/2, n+1) \int_0^1 \frac{p^{(n+1)-1}(1-p)^{(S+x_j+1/2)-1}}{B(S + x_j + 1/2, n+1)} dp \\
&= \frac{(x_j + 1/2)}{n} B(S + x_j + 1/2, n+1).
\end{aligned}$$

Summation over n such terms gives

$$\overline{m}_4^N(\boldsymbol{x}) = \frac{1}{n}\sum_{j=1}^{n} (x_j + 1/2)\, B(S + x_j + 1/2, n+1).$$

Computation

When both $\pi_i^N(\boldsymbol{\theta}_i \mid \boldsymbol{x}(l))$ and $\overline{m}_i^N(\boldsymbol{x})$ can be expressed in closed algebraic form then computation is straightforward. However, in general some form of numerical integration is usually required. Typically, it seems, the posterior distribution conditioned on the training sample, $\pi_i^N(\boldsymbol{\theta}_i \mid \boldsymbol{x}(l))$, can be expressed in some closed algebraic form and it is inevitably the pseudo-marginal density $\overline{m}_i^N(\boldsymbol{x})$ that requires numerical integration. Fortunately there are a plethora of suitable techniques that can be readily implemented.

Numerous methods exist for computing either $\pi_i^N(\boldsymbol{\theta}_i \mid \boldsymbol{x}(l))$ or $\overline{m}_i^N(\boldsymbol{x})$. In particular, standard quadrature integration can be usefully employed for low dimensional integration, and for integrations of higher dimension, Monte Carlo integration and the Metropolis algorithm are advantageous; see Kass and Raftery (1995), Smith and Gelfand (1992), Smith and Roberts (1993), Müller (1991), Berger and Pericchi (1996) and Gelfand, and Dey and Chang (1992) for discussion on this.

For the particular numerical example contained within this thesis, integration was conducted on $\overline{m}_2^N(\boldsymbol{x})$ over a using the trapezoidal rule, while the Metropolis algorithm (Müller, 1991) was used for the determination of $\overline{m}_3^N(\boldsymbol{x})$.

Results

The objective is to ascertain the most appropriate statistical density functions from the four candidate densities at each of the 35 sites. Model discrimination is also conducted on the hypothetical Site B data.

Results of the model discrimination made separately on the 35 accident sites using the averaged Bayes factor are presented in Table B.1 included in Appendix B. Coupled with the averaged Bayes factors, and also included in Table B.1, are the associated posterior probabilities of the four candidate models, derived using (3.3). Posterior probabilities were calculated assuming that all models were *a priori* equally likely, so that $P(M_1) = \ldots = P(M_4) = \frac{1}{4}$.

Table 3.2 summaries the results of these analyses pertaining to the 35 accident sites and reveals that; M_1 (the Poisson model) was the most preferred model on 22 occasions, M_2 (the Poisson/gamma model) was the most favoured at seven sites, and M_4 (the geometric density) appeared the most suitable at the remaining six sites. Interestingly, the mixture of two Poisson densities, M_3, was never preferred. Under

Table 3.2: Ranking frequencies of the four competing models at the 35 accident sites using the averaged Bayes factor discrimination technique.

Rank	M_1	M_2	M_3	M_4
1	22	7	0	6
2	4	28	2	1
3	2	0	31	2
4	7	0	2	26

this selection regime, M_2 was ranked second on 28 occasions, M_1 was second on four occasions, M_3 recorded the second highest posterior probability on two occasions while M_4 was ranked second at the remaining site.

To interpret the degree of superiority that the best model wields over the second ranked model we use the guidelines reported in Table 3.1. The evidence in favour of M_1, when it was best, compared to the second ranked model (which in all instances was M_2) was always *minimal*. Similarly, M_2, when best, was *minimally* better than the second ranked model on all seven occasions. Finally, in the six instances that M_4 was the best, evidence between it and the second ranked model (again, always M_2) was *positive* at Site 10 and *minimal* for the remaining five sites.

A notable feature of these analyses, as can be viewed from Table 3.2, was that the Poisson/gamma model never ranked lower than second of the four models under comparison. This is in contrast to the more frequently preferred Poisson model which ranked third at two sites and fourth (worst) at a further seven sites. Moreover, while the geometric model was *best* at six sites, it is apparent from Table 3.2 that the mixture of two Poisson distributions was the more generally preferred density of the two.

Averaging the posterior probability over all 35 sites gave $\overline{P}(M_1 \mid \boldsymbol{x}) = 0.313$, $\overline{P}(M_2 \mid \boldsymbol{x}) = 0.309$, $\overline{P}(M_3 \mid \boldsymbol{x}) = 0.230$, and $\overline{P}(M_4 \mid \boldsymbol{x}) = 0.148$, which suggests that while M_1 was more frequently preferred to M_2, it was not emphatically better. In terms of model discrimination for these data, it seems that, on average, the parsimony of the Poisson model gives it the slightest probabilistic edge over the less parsimonious but more flexible Poisson/gamma model. However, there are instances in which the Poisson distribution appears to perform badly comparative to the Poisson/gamma model. An investigation into each model's adequacy is thus required before either model can be globally adopted.

Binomial data

Results of the model discrimination based upon Site B data are presented in Table 3.3.

Table 3.3: Site B data: averaged Bayes factors and associated posterior probabilities (P_i denotes $P(M_i \mid \boldsymbol{x})$) for the four competing models.

Averaged Bayes factors						Posterior prob.			
B_{21}^A	B_{31}^A	B_{41}^A	B_{32}^A	B_{42}^A	B_{43}^A	P_1	P_2	P_3	P_4
0.373	0.305	2E–6	0.818	4E–6	5E–6	0.596	0.222	0.182	0.000

From these tabulated numbers it is evident that the averaged Bayes factor designated M_1 as being the best while M_2 was found to have the second highest posterior probability. The averaged Bayes factor comparing M_2 to M_1 was 0.373 which indicates that the Poisson density was *minimally* superior to the Poisson/gamma density.

This model discrimination saliently illustrates the statement made in Section 1.3.2

whereby Bayes factor strategies advocate superior models from the group under investigation, regardless of their fit. Had we not known that the data were binomial, and made no consideration of the adequacy of the Poisson model, we would have blithely proceeded with this discriminated model in subsequent analyses. Potentially, quite erroneous conclusions could have thus been drawn.

3.4.2 Bayes information criterion

For comparison, the approximation of the Bayes information criterion (3.11) was also applied on the same data to discriminate between the four competing models.

Computation

While maximum likelihood estimates (MLE) for the Poisson and geometric distributions are easily derived, estimates for the Poisson/gamma and mixture of Poisson distributions are not.

Maximum likelihood estimators for the Poisson/gamma model, which in effect gives rise to the negative binomial distribution, were obtained on solution of equations (30) and (31.1) on page 132 of Johnson and Kotz (1969), such that:

$$\widehat{a}\widehat{P} = \bar{x} \quad \text{and} \quad \log(1+\widehat{P}) = \sum_{j=1}^{\infty}(\bar{x}\widehat{P}^{-1} + j - 1)^{-1}F_j$$

where $F_j = \sum_{i=j}^{\infty} f_i$ = proportion of x which are greater than or equal to j and $\widehat{P} = (1-\widehat{p})/\widehat{p}$.

Instances arise, however, when the MLE does not exist (due to the data being under-dispersed) in which case parameters were calculated assuming that the sample variance was ϵ larger than the sample mean, where ϵ is some small number (in this case 1E–10). This implies that $\widehat{p} = \bar{x}/(\bar{x}+\epsilon)$ and $\widehat{a} = \bar{x}\widehat{p}/(1-\widehat{p})$.

The maximum likelihood estimates for the mixture of two Poisson densities are also not explicitly solvable for the parameters of interest, necessitating the use of iterative techniques. Everitt and Hand (1981) derive such a system of equations with

$$\widehat{p}_i = \frac{1}{n}\sum_{j=1}^{n}\widehat{P}(i \mid X_j)$$

$$\widehat{\lambda}_i = \frac{1}{n\widehat{p}_i}\sum_{j=1}^{n}X_j\,\widehat{P}(i \mid X_j)$$

where

$$\widehat{P}(i \mid X_j) = \frac{\widehat{p}_i \, P_i(x \mid \widehat{\lambda}_i)}{P(x \mid \widehat{\boldsymbol{p}}, \widehat{\boldsymbol{\lambda}})}$$

for $\widehat{\boldsymbol{\lambda}} = (\widehat{\lambda}_1, \widehat{\lambda}_2)$ and $\widehat{\boldsymbol{p}} = (\widehat{p}_1, \widehat{p}_2)$. Note here that $\widehat{p}_2 = 1 - \widehat{p}_1$. Given initial values for $\widehat{\boldsymbol{\lambda}}$ and $\widehat{\boldsymbol{p}}$, these equations can be used to form the basis for this iterative estimation algorithm. Unfortunately a deficiency of this iterative technique, common with many such algorithms, is that different initial values may lead to widely different final estimates. All resultant estimates were thus verified using the Newton-Raphson algorithm and checks on the value of the likelihood function.

Results

Table B.2 contained in Appendix B houses the results from implementation of (3.11). Associated posterior probabilities, derived using (3.3), are also included in this table. Again, these posterior probabilities were calculated assuming *a priori* that each model was equally likely.

Perusal of these calculations, which have been summarised in Table 3.4, reveal that M_1 was best at 26 sites (up four from the number designated by the averaged Bayes factor), M_2 was best at two sites (down five), M_4 was best at seven sites (up one), while M_3 was never superior (as before).

Table 3.4: Ranking frequencies of the four competing models at the 35 accident sites using the approximated BIC discrimination method.

Rank	M_1	M_2	M_3	M_4
1	26	2	0	7
2	3	25	0	7
3	3	8	16	8
4	3	0	19	13

Although infrequently the best model, M_2 was ranked second on 25 occasions, M_1 was second on three occasions, while M_4 was ranked second at the remaining seven sites. Notably, M_3 was never selected within the top two of the four models studied for any site. Again using the discrimination strengths of Table 3.1, evidence in favour of M_1, when it was best, compared to the second ranked model was in 15 instances *positive* and on a further eleven occasions *minimal*. M_2 was *minimally*

better than the second ranked model on each of the two occasions it was best. Finally, in the seven instances that M_4 was the best, evidence between it and the second ranked model was *positive* on two occasions and *minimal* for the remaining five sites.

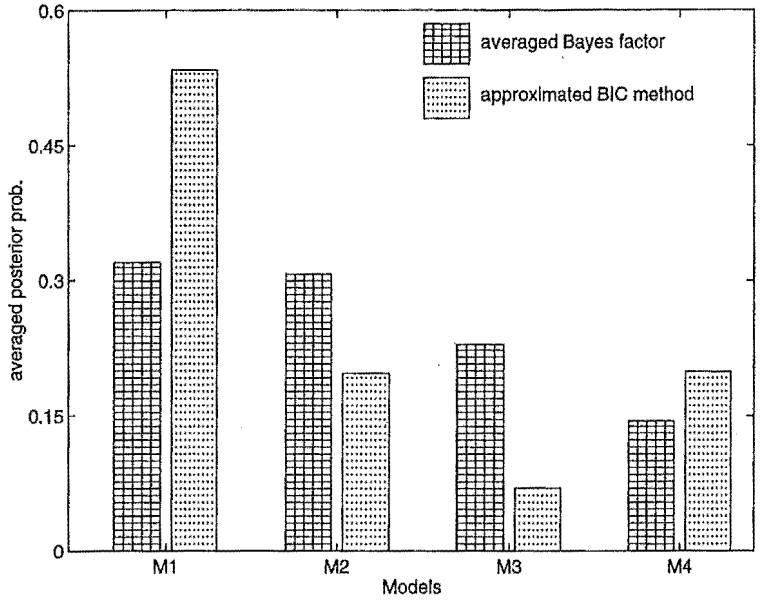
While some degree of consistency emerged between the best models designated by the two considered discrimination techniques, the weight of evidence for the simpler models was considerably less with adoption of the averaged Bayes factor method. This systematic trend was revealed when results compiled in Table 3.2 and Table 3.4 were directly compared. When utilising the approximated BIC criterion (Table 3.4) after the averaged Bayes factor discrimination method (Table 3.2) a general improvement in rankings for the Poisson and geometric models and, correspondingly, a deterioration in both the Poisson/gamma and Poisson mixtures rankings was clearly evident.

Averaging the posterior probabilities derived using the approximated BIC method over the 35 sites yielded $\overline{P}(M_1 \mid \boldsymbol{x}) = 0.534$, $\overline{P}(M_2 \mid \boldsymbol{x}) = 0.197$, $\overline{P}(M_3 \mid \boldsymbol{x}) = 0.070$, and $\overline{P}(M_4 \mid \boldsymbol{x}) = 0.199$. These averages suggest that not only was M_1 often superior to the other candidates but it was superior with considerably higher probability.

Another notable feature of these averaged probabilities was the magnitude of support given to the geometric model by the approximated BIC discrimination method. Indeed, according to the averaged posterior probabilities reported above, the geometric density surpassed the Poisson/gamma in terms of model preference, albeit with a small 0.002 probability margin.

These numerical characteristics are illustrated in Figure 3.1 which presents the averaged posterior probabilities for each candidate model by the two model discrimination techniques considered. Observe from this figure that the averaged posterior probability for M_1 using the approximated BIC technique was $\overline{P}(M_1 \mid \boldsymbol{x}) = 0.534$, a value considerably higher than the averaged probability using the averaged Bayes factor method with $\overline{P}(M_1 \mid \boldsymbol{x}) = 0.313$. Similiarly, the simpler geometric model M_4 had, on average, higher probability with the adoption of the approximated BIC discrimination procedure; $\overline{P}(M_4 \mid \boldsymbol{x}) = 0.199$ versus 0.148, respectively. Correspondingly, both the more complex models, M_2 and M_3, had lower averaged posterior probabilities for the approximated BIC procedure compared to the averaged Bayes factor method.

Figure 3.1: Averaged posterior probabilities $\overline{P}(M_i \mid \boldsymbol{x})$, $i = 1, 2, 3$ and 4, derived from the averaged Bayes factor and approximated BIC method over the 35 accident sites.



The increased support for the Poisson model by the approximated BIC method, compared to the averaged Bayes factor, is illustrated for each individual site in Figure 3.2. In this figure, the extent of the increased support for the Poisson model by the approximated BIC method has been depicted by the dotted lines. This figure quite dramatically demonstrates the previously described inherent failing of the BIC approach, in this case favouring the simpler model when the sample size was small.

Binomial data

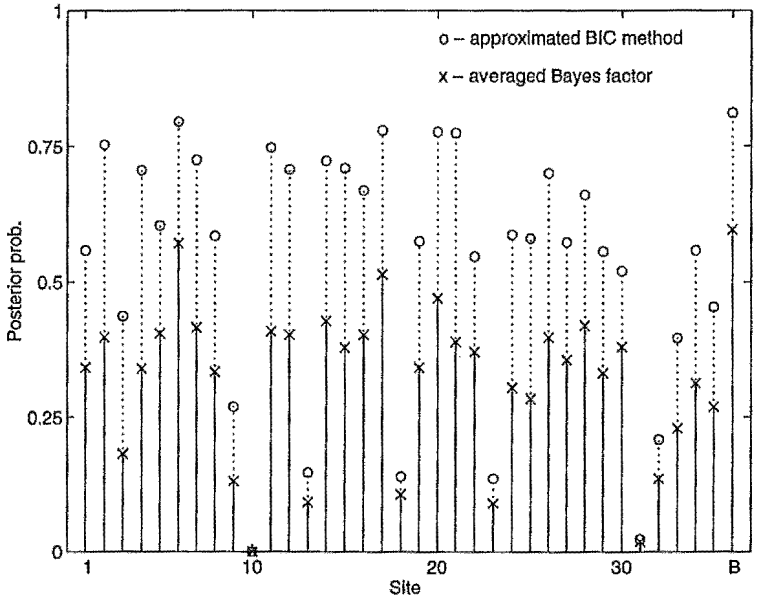
Increased support by the BIC method for the simplier model was also evident when the hypothetical data were analysed, as can be seen in Table 3.5. Calculations

Table 3.5: Site B data: approximated BIC Bayes factors and associated posterior probabilities (P_i denotes $P(M_i \mid \boldsymbol{x})$) for the four competing models.

approximated BIC Bayes factors						Posterior prob.			
B^S_{21}	B^S_{31}	B^S_{41}	B^S_{32}	B^S_{42}	B^S_{43}	P_1	P_2	P_3	P_4
0.224	0.010	2E–6	0.044	7E–6	2E–4	0.811	0.181	0.008	0.000

based on the hypothetical data revealed that M_1 was best and that M_2 was, again,

Figure 3.2: Posterior probabilities for the Poisson model at each of the 35 accident sites and at Site B derived from the averaged Bayes factor (denoted by '×') and the approximated BIC method (denoted by 'o').



the second most suitable model of the four. Using the guidelines of Table 3.1, the comparison of M_2 to M_1 resulted in the Poisson model being *positively* better with $B_{21}^S = 0.224$.

To recapitulate, model discrimination made using a Bayes factor (or the Bayes factor principle) is primarily based on the comparative likelihood of two models explaining the data. Discrimination made in this fashion accurately assesses and differentiates between competing models, advocating *best* model(s), but makes no explicit statement concerning the compatibility of the best model(s) with the data.

In the hypothetical Site B scenario, data were deliberately generated from a fully specified and under-dispersed distribution that was entirely inconsistent from those models being investigated. Almost certainly, all four candidate models would poorly represent these data yet both model discrimination strategies selected the Poisson distribution. Clearly the Poisson model is genuinely superior to the other three distributions considered, but could it be used to adequately describe this hypothetical accident data? This question provides the motivation for the next chapter.

Chapter 4

Model Adequacy and Power

The proposed averaged Bayes factor technique discriminates by simply *comparing* models. Having differentiated between a group of models using such a technique, it may be tempting to simply choose a particular M_j because it performed "the best" for the given data amongst the κ competing models. However, model selection made in this fashion ignores the important question of: "Is M_j *consistent* enough with the observed data for us to confidently use such a model?". Only further examination of the preferred model can suitably answer this question.

In this chapter we assume that the analyst, through some appropriate means, has discriminated and identified what they consider to be the best density M_j. The analyst, wanting to answer the important question and confirm the applicability of M_j, must then test its compatibility with the observed data. That is, the analyst must ascertain whether the *empirical data are likely to have originated from this chosen model.* If the observed data had little chance of arising from M_j then its appropriateness must be seriously questioned, as such a model is unlikely to provide accurate or useful information for ensuing inferences.

4.1 Preliminaries

Suppose that the distributional function M_j is discriminated from a pool of candidate densities $M_1, \ldots, M_\kappa$ to best represent some conditionally independent vector of data $\boldsymbol{x} = (x_1, \ldots, x_n)$. Selection of model M_j implies x_i is assumed to be distributed by $f_j(x_i \mid \boldsymbol{\theta}_j)$ hence the data are conditional upon some h_j–dimensional vector of unknown parameters $\boldsymbol{\theta}_j$.

Posterior distribution

If $\pi_j(\boldsymbol{\theta}_j)$ represents some informative or noninformative (dropping the superscript N) prior distribution for $\boldsymbol{\theta}_j$, then, as we have seen in (3.4), the posterior distribution of $\boldsymbol{\theta}_j$ is given by the h_j–dimensional integral

$$\pi_j(\boldsymbol{\theta}_j \mid \boldsymbol{x}) = \frac{f_j(\boldsymbol{x} \mid \boldsymbol{\theta}_j)\, \pi_j(\boldsymbol{\theta}_j)}{\int f_j(\boldsymbol{x} \mid \boldsymbol{\theta}_j)\, \pi_j(\boldsymbol{\theta}_j)\, d\boldsymbol{\theta}_j} \tag{4.1}$$

where

$$f_j(\boldsymbol{x} \mid \boldsymbol{\theta}_j) = \prod_{i=1}^{n} f_j(x_i \mid \boldsymbol{\theta}_j).$$

Posterior predictive distribution

Using a similar rationale to Gelman *et al.* (1995), we define the random variable $\boldsymbol{Y}$ as the *replicated data* that *could have been* observed, or, in the predictive sense, as the data we *would* see over the next n years if the circumstances that produced $\boldsymbol{x}$ over the last n years were repeated with the same model and underlying accident rate $\boldsymbol{\theta}$. Specifically, $\boldsymbol{y}$ is a replication just like $\boldsymbol{x}$.

The predictive distribution corresponding to M_j for the vector of unobserved random variables, $\boldsymbol{Y}$, denoted by $f_j(\boldsymbol{y} \mid \boldsymbol{x})$, can then be given by

$$f_j(\boldsymbol{y} \mid \boldsymbol{x}) = \int f_j(\boldsymbol{y} \mid \boldsymbol{\theta}_j, \boldsymbol{x})\, \pi_j(\boldsymbol{\theta}_j \mid \boldsymbol{x})\, d\boldsymbol{\theta}_j. \tag{4.2}$$

As the data are assumed to be conditionally independent, (4.2) can be simplified to

$$f_j(\boldsymbol{y} \mid \boldsymbol{x}) = \int f_j(\boldsymbol{y} \mid \boldsymbol{\theta}_j)\, \pi_j(\boldsymbol{\theta}_j \mid \boldsymbol{x})\, d\boldsymbol{\theta}_j. \tag{4.3}$$

Gelman *et al.* (1995), and we hereafter, refer to (4.3) as the *posterior predictive distribution*. This nomenclature arises naturally by noting that the prediction vector

of future observables $\boldsymbol{y}$ is condition on $\boldsymbol{\theta}_j$ which is distributed by the posterior distribution $\pi_j(\boldsymbol{\theta}_j \mid \boldsymbol{x})$.

The cumulative distribution function of $f_j(\boldsymbol{y} \mid \boldsymbol{x})$ under the hypothesised model M_j is denoted by $F_j(\boldsymbol{y} \mid \boldsymbol{x})$.

Hold-out predictive distribution

Cross-validation works on the principle that successive observations x_i, $i = 1, \ldots, n$, are singly held out of a sample thereby allowing the remaining $n-1$ observations $\boldsymbol{x}_{(i)} = (x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n)$ to determine a hold-out predictive density denoted by $f_j(x_i \mid \boldsymbol{x}_{(i)})$. Cross-validation calculations then ensue by employing various measures to assess the likelihood of each x_i originating from $f_j(x_i \mid \boldsymbol{x}_{(i)})$.

The hold-out predictive density is defined by

$$f_j(x_i \mid \boldsymbol{x}_{(i)}) = \int f_j(x_i \mid \boldsymbol{\theta}_j)\, \pi_j(\boldsymbol{\theta}_j \mid \boldsymbol{x}_{(i)})\, d\boldsymbol{\theta}_j, \tag{4.4}$$

for a particular selected model M_j when the data are assumed to be conditionally independent. The mean and variance of this predictive density (4.4) are denoted by $\mu_{j(i)} = \mathrm{E}_j[X_i \mid \boldsymbol{x}_{(i)}]$ and $\sigma^2_{j(i)} = var_j(X_i \mid \boldsymbol{x}_{(i)})$, respectively.

4.2 Adequacy measures and their assessment

The strategy is to assess, under some assumed model M_j, the ability of distributions (4.3) in forecasting and (4.4) in representing the observed data which have been held out of the sample. This assessment can be accomplished using various *adequacy measures*.

Three measures offered by Gelfand, Dey and Chang (1992) and Upadhyahy and Smith (1993) are conducive to the simulation approach suggested within this thesis. Other measures exist or could be constructed but, for brevity, only these three choices of model adequacy will be reported.

1. Let $\mathcal{D}^1(M_j) = \sum_{i=1}^n (x_i - \mu_{j(i)})^2 / \sigma^2_{j(i)}$, the summed squared standardised residual for each held out observation x_i assuming model M_j.

2. Let $\mathcal{D}^2(M_j) = \prod_{i=1}^n f_j(x_i \mid \boldsymbol{x}_{(i)})$, the product of the predictive likelihoods for each held out observation x_i assuming model M_j.

3. Let $\mathcal{D}^3(M_j) = \sup_t \mid \widehat{F}_n(t) - F_j(t \mid \boldsymbol{x}) \mid$, the Kolmogorov-Smirnov measurement of discrepancy under model M_j, where $\widehat{F}_n(t)$ is the empirical cumulative frequency distribution given by

$$\widehat{F}_n(t) = \frac{\text{number of } x_i\text{'s } \leq t}{n}.$$

For a data sequence $\boldsymbol{x} = (x_1, \ldots, x_n)$ and discriminated model M_j, answers to the question "is this identified model adequate?" can be achieved using adequacy measures $\mathcal{D}^r(M_j)$.

While $\mathcal{D}^1$, $\mathcal{D}^2$ and $\mathcal{D}^3$ are all complicated functions of the data they possess two important properties: they have intuitive appeal and are readily computed. The $\mathcal{D}^1$ statistic measures the standardised squared deviations from the mean (similar to summed squared residuals and chi-squared goodness-of-fit statistics) in a fashion similar to the PRESS statistic recommended by Allen (1971); $\mathcal{D}^2$ represents the product of predictive probabilities, a statistic introduced by Geisser and Eddy (1979); while $\mathcal{D}^3$ measures the compatibility between the empirical data and its associated predictive distribution under some model. These are standard and frequently employed goodness-of-fit measures.

To make any quantitative judgement based on the observed adequacy measurement, the statistical distribution of that adequacy measure when the assumed model M_j is *true* is required. This statistical distribution provides the *frame of reference* or, more simply, the type of $\mathcal{D}^r$ values that can be expected under M_j. Once ascertained, the observed adequacy measurement can be compared to the distribution of measures expected under M_j so that an assessment of the assumed model's adequacy can be made.

If the observed adequacy measurement falls in the tails of its associated distribution of expected adequacy measures, then the likelihood of the observed adequacy measurement originating from that distribution is small. This, in turn, implies that it is unlikely that the empirical data giving rise to this observed adequacy measurement could have originated from the assumed model. Alternatively, if the observed adequacy measurement was embodied within the anticipated range of its associated distribution of expected measures, then no evidence exists to question the origin of the observed adequacy measurement. This, in turn, implies that there is no reason to doubt the validity of the assumed model.

Before these ideas can be statistically expressed, some additional notation is required. The observed adequacy measurement based upon some measure $\mathcal{D}^r(M_j)$, observed data $\boldsymbol{x}$ and assumed model M_j, is denoted by $d^r(M_j)$. Let $D_i^r(M_j, M_k)$ represent the value derived from applying the $\mathcal{D}^r(M_j)$ adequacy measure to some data vector $\boldsymbol{y}_i$ which orginated (as discussed later) from some underlying model M_k. The distribution of $D_i^r(M_j, M_k)$ values is denoted by $\mathcal{F}^r(d \mid j, k)$, and the symbol $D^r(M_j, M_k)$ is used to denote a random variable from $\mathcal{F}^r(d \mid j, k)$.

For any observed adequacy measurement $d^r(M_j)$ we are interested in determining its expected statistical distribution when M_j is *true*; that is, we seek $\mathcal{F}^r(d \mid j, j)$, the distribution of $D^r(M_j, M_j)$ values. Once this distribution has been derived, critical values can be ascertained and compared with the observed adequacy measurement $d^r(M_j)$. For any specified α level, critical values $c_\alpha^r(M_j)$ are defined by

$$P\left(D^r(M_j, M_j) \geq c_{1-\alpha}^r(M_j)\right) \leq \alpha \tag{4.5}$$

or

$$\begin{cases} P\left(D^r(M_j, M_j) \leq c_{\alpha/2}^r(M_j)\right) \leq \frac{\alpha}{2} \\ \text{and} \\ P\left(D^r(M_j, M_j) \geq c_{1-\alpha/2}^r(M_j)\right) \leq \frac{\alpha}{2} \end{cases} \tag{4.6}$$

depending on the one-sided or two-sided nature of the rejection regions, respectively.

Should the investigation into M_j's adequacy be made using a one-sided rejection region, then (4.7) defines the appropriate decision rule once critical values $c_{1-\alpha}^r(M_j)$ have been ascertained from $\mathcal{F}^r(d \mid j, j)$.

$$\begin{gathered} \textit{Reject} \text{ the adequacy of } M_j \text{ iff } d^r(M_j) \geq c_{1-\alpha}^r(M_j), \\ \text{otherwise } \textit{accept} \text{ the adequacy of } M_j. \end{gathered} \tag{4.7}$$

If $d^r(M_j) \geq c_{1-\alpha}^r(M_j)$ then, using conventional statistical logic, $d^r(M_j)$ is deemed unlikely to have arisen from $\mathcal{F}^r(d \mid j, j)$, at level α. Moreover, this implies that the likelihood of the observed data originated from selected model M_j is small thereby questioning this model's adequacy.

Similarly, should the examination of M_j's adequacy be conducted using two-sided rejection regions, then (4.8) defines the appropriate decision rule.

$$\textit{Reject} \text{ the adequacy of } M_j \text{ iff } \begin{cases} d^r(M_j) \leq c^r_{\alpha/2}(M_j) \\ \text{or} \\ d^r(M_j) \geq c^r_{1-\alpha/2}(M_j), \end{cases} \tag{4.8}$$

otherwise *accept* the adequacy of M_j.

Again, $c^r_{\alpha/2}(M_j)$ and $c^r_{1-\alpha/2}(M_j)$ are critical values derived from $\mathcal{F}^r(d \mid j, j)$.

The approach of (4.7) and (4.8) implies that if the predictive distribution of the assumed underlying model is able to accurately mimic the observed data, then we anticipate that the observed adequacy measures $d^r(M_j)$ would be contained within those regions given high probability by $\mathcal{F}^r(d \mid j, j)$. However, models yielding predictive distributions that fail to reproduce data similar to that observed would result in observed adequacy measures $d^r(M_j)$ lying on the extremities of the associated $D^r(M_j, M_j)$ distributions. Consequently, a model M_j is deemed to be inadequate for measure $\mathcal{D}^r$ at the α significance level if $d^r(M_j)$ is rejected by either (4.7) or (4.8), which ever is the appropriate decision rule. The pre-specified α value is simply the usual significance level.

For the situation described herein, adequacy measure distributions $\mathcal{F}^1(d \mid j, j)$ and $\mathcal{F}^2(d \mid j, j)$ are both assumed to have two-sided rejection regions. This arises since alternative densities exist that generate data $\boldsymbol{x}$ such that values of $d^1(M_j)$ and $d^2(M_j)$ are generally both lower or higher than can be expected when M_j is actually true. This implies that both low and high $d^1(M_j)$ and $d^2(M_j)$ values are indicative of an alternative rather than the incumbent selected model. Appropriate model adequacy discrimination thereby requires the specification of two-sided rejection regions as given by (4.6) and (4.8).

However, for the $\mathcal{D}^3$ Kolmogorov-Smirnov adequacy measure, it is unknown whether reasonable alternative probability distributions exist that generate data $\boldsymbol{x}$ such that the values of the $d^3(M_j)$ statistic are generally lower than can be expected from $\mathcal{F}^3(d \mid j, j)$. An alternative distribution of this type would have to generate data with frequency closer to the assumed predictive distribution than could be expected to be generated from that predictive distribution itself. Apart from deterministic distributions, it seems that such distributions would, in practice, rarely exist and therefore the one-sided rejection regions, defined by (4.5) and (4.7),

appear entirely appropriate.

The one-sided and two-sided nature of the rejection regions for these adequacy measures will be discussed further in Section 4.5.

4.3 Power of adequacy measures

The power of an adequacy test is defined to be the probability that the selected model M_j is deemed inadequate when $\boldsymbol{x}$, in actuality, arose from some alternative density function. Calculations of power are useful for determining the sensitivity of a particular $\mathcal{D}^r$ measure in identifying data that are not consistent with the assumed underlying model.

Statistically, the power of the adequacy measure $\mathcal{D}^r$ under model M_j when the alternative M_k is actually the underlying generating function, is defined for the one-sided test by

$$P^r(M_j, M_k) = 1 - P\left(D^r(M_j, M_k) < c^r_{1-\alpha}(M_j)\right), \tag{4.9}$$

and for two-sided test by

$$P^r(M_j, M_k) = 1 - P\left(c^r_{\alpha/2}(M_j) < D^r(M_j, M_k) < c^r_{1-\alpha/2}(M_j)\right). \tag{4.10}$$

For this calculation to be conceptually meaningful, the alternative density function M_k must be generally consistent or adequate with the accident data commonly observed. It makes no intuitive sense to estimate the probability that a particular distribution will be found to be inadequate, conditional upon some alternative model M_k that itself is entirely inconsistent with the observed empirical data. Power estimates should be based upon those alternative distributions that are themselves generally adequate or that are likely to be compatible with the data.

To carry out our proposed assessment of adequacy for some particular model M_j, appropriate distributions for both $\mathcal{F}^r(d \mid j, j)$ and $\mathcal{F}^r(d \mid j, k)$ must be determined, at least to the extent that calculations of (4.5), (4.6), (4.9) and (4.10) are possible. This will be accomplished in the next section using Monte Carlo simulation.

4.4 Simulation approach

Through simulation the practitioner is empowered with a method that quantitatively measures whether observed adequacy measurements are consistent with the selected model.

Conditional upon a set of observed data $\boldsymbol{x} = (x_1, \ldots, x_n)$, a selected model M_j and some measure of adequacy $\mathcal{D}^r$, our recommended simulation scheme takes the following course.

1. Evaluate the observed adequacy measurement value $d^r(M_j)$.
2. Generate N observations of *replicated data* $\{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_N\}$, each $\boldsymbol{y}_i$ being an n vector generated from the posterior predictive distribution $f_j(\boldsymbol{y} \mid \boldsymbol{x})$.
3. For the N values of $\boldsymbol{y}_i$ compute associated $D_i^r(M_j, M_j)$ values.
4. Compile an ordered list of $D_i^r(M_j, M_j)$ values, forming $\widehat{\mathcal{F}}^r(d \mid j, j)$, and hence obtaining critical values $\widehat{c}_\alpha^r(M_j)$.
5. Determine model M_j's adequacy using either (4.7) or (4.8), whichever is appropriate.

Suppose, using some measure $\mathcal{D}^r$, that the power of finding M_j inadequate when the data arose from model M_k is now required. That is, it is necessary to estimate $P^r(M_j, M_k)$. Estimates of power can be determined in a similar fashion to the simulation scheme presented above. The manner in which this can be done now follows.

Having previously performed Steps 1–5 above, $\widehat{P}^r(M_j, M_k)$ can be estimated (using either (4.9) or (4.10), whichever is appropriate) by repeating Step 2 except replacing $f_j(\boldsymbol{y} \mid \boldsymbol{x})$ with $f_k(\boldsymbol{y} \mid \boldsymbol{x})$. Application of the posterior predictive distribution $f_k(\boldsymbol{y} \mid \boldsymbol{x})$ ensures that the generated N observations of replicated data will be acquired from M_k. Next, Step 3 should also be repeated except that now $D_i^r(M_j, M_k)$ will be computed as the N values of replicated data were acquired from M_k and not M_j. Finally, an estimate of power can be attained by counting Q the number of instances $D_i^r(M_j, M_k) < \widehat{c}_{1-\alpha}^r(M_j)$, for a one-sided adequacy test, or $\widehat{c}_{\alpha/2}^r(M_j) < D_i^r(M_j, M_k) < \widehat{c}_{1-\alpha/2}^r(M_j)$, for a two-sided adequacy test, and then assigning $\widehat{P}^r(M_j, M_k) = 1 - Q/N$.

Upon first impression it may appear that this suggested technique uses the observed data twice, namely in Steps 1 and 2, something contrary to the traditional Bayesian logic. Certainly, $d^r(M_j)$ can only be constructed using the observed data so it is the use of $f_j(\boldsymbol{y} \mid \boldsymbol{x})$ and $f_k(\boldsymbol{y} \mid \boldsymbol{x})$ that may appear questionable. We opine, however, that the employment of these posterior predictive distributions conditioned upon the observed data $\boldsymbol{x}$ is perfectly reasonable. Our justification for this stance is based on the following rationale.

The primary objective in determining model adequacy is to ascertain whether the *best* members contained within the family of parameters for a model under investigation can adequately describe the data. That is, model assessment should be made by examining the compatibility between the empirical observations and the specification of the model which is most consistent with those observed data. From a Bayesian perspective, our *best* understanding of future observations is derived from the predictive distribution (Box, 1980, Berger, 1985, Rubin, 1984). This implies that it is both coherent and sensible to employ the predictive distribution conditioned upon the observed data for the determination of adequacy distributions, critical values, adequacy interpretations and power estimates, as proposed in this chapter. Furthermore, data have been used in this fashion previously (Upadhyahy and Smith, 1993, Gelman *et al.*, 1995).

4.5 Numerical details

The objective is to examine the adequacy of those models deemed as being the *best*, identified using the averaged Bayes factor in Section 3.4. In particular, the global adequacy of the Poisson and Poisson/gamma models needs investigation. Before this can be undertaken, mathematical details of the posterior predictive distribution and the hold-out predictive distribution for the four candidate models requires attention.

4.5.1 Posterior predictive distributions

The posterior predictive distributions are used to generate the replicate data. Recall that these replicate data are, in essence, predictive data that we would see over the next n years if the circumstances were unchanged from the last n years when $\boldsymbol{x}$ were observed.

The complicated nature of the posterior predictive distributions defined by (4.3) makes it difficult to directly acquire replicate data from these densities. Instead, simulation is required to generate such data. Fortunately, this technique can easily be accommodated into the simulation scheme developed in the preceding section.

In Step 2 of Section 4.4, we required the generation of N observations of *replicated data* $\{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_N\}$, each $\boldsymbol{y}_i$ being an n vector generated from the posterior predictive distribution $f_j(\boldsymbol{y} \mid \boldsymbol{x})$. Using the method of Gelman *et al.* (1995), this can be easily accomplished by initially drawing N values of $\boldsymbol{\theta}_j$ from the posterior distribution $\pi_j(\boldsymbol{\theta}_j \mid \boldsymbol{x})$, given by (4.1). We denote these drawn $\boldsymbol{\theta}_j$ values by $\boldsymbol{\theta}_j^i$ for $i = 1, \ldots, N$. Once drawn, we then generate one $\boldsymbol{y}_i$ vector from the predictive distribution for each simulated $\boldsymbol{\theta}_j^i$. The predictive distribution is given by $f_j(\boldsymbol{y} \mid \boldsymbol{\theta}_j^i, \boldsymbol{x}) = f_j(\boldsymbol{y} \mid \boldsymbol{\theta}_j^i)$ when the data are assumed to be conditionally independent. Acquisition of conditionally independent data from $f_j(\boldsymbol{y} \mid \boldsymbol{\theta}_j^i)$ is easily achieved as this predictive distribution is fully specified. This technique thus provides the N observations of replicate data generated from $f_j(\boldsymbol{y} \mid \boldsymbol{x})$ required by our simulation scheme.

However, before the proposed simulation scheme can be implemented, we need to the specify the posterior distributions (4.1) for the four models under investigation and verify that they are defined. These posterior distributions are now considered.

Posterior distribution: $\pi_1(\boldsymbol{\theta}_1 \mid \boldsymbol{x})$

The posterior distribution for M_1 has denominator given by

$$\begin{aligned} \int f_1(\boldsymbol{x} \mid \boldsymbol{\theta}_1)\, \pi_1(\boldsymbol{\theta}_1)\, d\boldsymbol{\theta}_1 &= \int_0^\infty \left[\prod_{i=1}^n \frac{\lambda^{x_i} e^{-\lambda}}{x_i!}\right] \frac{1}{\sqrt{\lambda}}\, d\lambda \\ &= \left[\prod_{i=1}^n \frac{1}{x_i!}\right] \int_0^\infty \lambda^{S-1/2} e^{-n\lambda} d\lambda \end{aligned}$$

where, as before, $S = \sum_{i=1}^n x_i$. Recognising the form of the gamma distribution, providing $n > 0$ and $S + 1/2 > 0$, this integral can be rewritten by

$$\left[\prod_{i=1}^n \frac{1}{x_i!}\right] \frac{\Gamma(S+1/2)}{n^{S+1/2}} \int_0^\infty \frac{n^{S+1/2}}{\Gamma(S+1/2)} \lambda^{(S+1/2)-1} e^{-n\lambda} d\lambda$$

which simplifies to

$$\left[\prod_{i=1}^n \frac{1}{x_i!}\right] \frac{\Gamma(S+1/2)}{n^{S+1/2}}$$

and so the posterior distribution can be expressed by the gamma density

$$\pi_1(\boldsymbol{\theta}_1 \mid \boldsymbol{x}) = \frac{n^{S+1/2}}{\Gamma(S+1/2)} \lambda^{(S+1/2)-1} e^{-n\lambda}. \tag{4.11}$$

which is proper for $x_i \geq 0$ and $n \geq 1$.

Posterior distribution: $\pi_2(\boldsymbol{\theta}_2 \mid \boldsymbol{x})$

The marginal distribution of $\boldsymbol{x}$ for M_2 can be expressed by

$$\begin{aligned} \int f_2(\boldsymbol{x} \mid \boldsymbol{\theta}_2)\, \pi(\boldsymbol{\theta}_2)\, d\boldsymbol{\theta}_2 &= \int_0^1 \int_0^\infty \left[\prod_{i=1}^n \binom{x_i + a - 1}{x_i} p^a (1-p)^{x_i} \right] \frac{1}{\sqrt{a+1}}\, da\, dp \\ &= \int_0^\infty \left[\prod_{i=1}^n \binom{x_i + a - 1}{x_i} \right] \frac{1}{\sqrt{a+1}} \int_0^1 p^{na} (1-p)^S\, dp\, da. \end{aligned}$$

Recognising the form of the beta distribution, providing $na + 1 > 0$ and $S + 1 > 0$, this integral can be rewritten as

$$\int_0^\infty \left[\prod_{i=1}^n \binom{x_i + a - 1}{x_i} \right] \frac{B(S+1, na+1)}{\sqrt{a+1}} \int_0^1 \frac{p^{(na+1)-1}(1-p)^{(S+1)-1}}{B(S+1, na+1)}\, dp\, da$$

which simplifies to

$$\int_0^\infty \left[\prod_{i=1}^n \binom{x_i + a - 1}{x_i} \right] \frac{B(S+1, na+1)}{\sqrt{a+1}}\, da.$$

Therefore, the posterior distribution for M_2 requires one-dimensional integration over a, and can be expressed by

$$\pi_2(\boldsymbol{\theta}_2 \mid \boldsymbol{x}) = \frac{\left[\prod_{i=1}^n \binom{x_i + a - 1}{x_i} \right] \frac{p^{na}(1-p)^S}{\sqrt{a+1}}\, da}{\int_0^\infty \prod_{i=1}^n \binom{x_i + a - 1}{x_i} \frac{B(S+1, na+1)}{\sqrt{a+1}}\, da}. \tag{4.12}$$

It is straight forward to prove that (4.12) gives a defined and proper integral over a and p for all $x_i \geq 0$, $y \geq 0$ and $n \geq 1$. To show this, it is sufficient to prove that the denominator is defined and bounded away from 0 and ∞.

Let R denote the denominator of (4.12). After expansion, note that

$$R = C \int_0^\infty \frac{\prod_{i=1}^n [(x_i + a - 1)((x_i - 1) + a - 1) \ldots (0 + a - 1)]}{[((S+1) + na)(S + na) \ldots (1 + na)]\, (a-1)^n \sqrt{a+1}}\, da$$

$$\leq C \int_0^\infty \frac{(x_{\max} - 1 + a)^S}{(a+1)^{S+3/2}}\, da$$

$$= C \int_0^\infty \left(\frac{x_{\max} - 1 + a}{a+1}\right)^S \frac{1}{(a+1)^{3/2}}\, da$$

where $C = \Gamma(S+1)\,[\prod_{i=1}^n x_i!]^{-1}$ and $x_{\max} = \max(x_1, \ldots, x_n)$. Now, for any $x_{\max} \geq 0$ and $a > 0$, it can be observed that $(x_{\max} - 1 + a)/(a+1) \leq (x_{\max} + 1)$. Hence

$$C \int_0^\infty \left(\frac{x_{\max} - 1 + a}{a+1}\right)^S \frac{1}{(a+1)^{3/2}}\, da \leq C \int_0^\infty \frac{(x_{\max}+1)^S}{(a+1)^{3/2}}\, da$$

$$= C\,(x_{\max}+1)^S \int_0^\infty \frac{1}{(a+1)^{3/2}}\, da$$

$$= 2\,\Gamma(S+1) \left[\prod_{i=1}^n \frac{1}{x_i!}\right] (x_{\max}+1)^S,$$

and thus $R < \infty$. A similar approach can be exploited to establish a minimum bound for R that is bounded above 0, by noting that

$$R \geq C \int_0^\infty \frac{1}{((S+1) + na)^{S+3/2}}\, da.$$

These finite and non-zero bounds ensure that $\pi_2(\boldsymbol{\theta}_2 \mid \boldsymbol{x})$ is proper for $x_i \geq 0$ and $n \geq 1$.

Posterior distribution: $\pi_3(\boldsymbol{\theta}_3 \mid \boldsymbol{x})$

The posterior distribution for M_3 can not easily be simplified from

$$\pi_3(\boldsymbol{\theta}_3 \mid \boldsymbol{x}) = \frac{\left[\prod_{i=1}^n \frac{p\lambda_1^{x_i} e^{-\lambda_1}}{x_i!} + \frac{(1-p)\lambda_2^{x_i} e^{-\lambda_2}}{x_i!}\right] \frac{1}{\lambda_2^{3/2}}}{\int\int\int \left[\prod_{i=1}^n \frac{p\lambda_1^{x_i} e^{-\lambda_1}}{x_i!} + \frac{(1-p)\lambda_2^{x_i} e^{-\lambda_2}}{x_i!}\right] \frac{1}{\lambda_2^{3/2}}\, dp\, d\lambda_1\, d\lambda_2} \tag{4.13}$$

where $0 < p < 1$ and $0 < \lambda_1 < \lambda_2 < \infty$. Despite this, it is relatively easy to verify that this distribution is proper for all $x_i \geq 0$ and $n \geq 1$ over p, λ_1 and λ_2.

Again, to prove that this distribution is proper, it is sufficient to show that the denominator is defined and bounded away from 0 and ∞. Let R denote the denominator of (4.13). After expansion, it is clear that

$$R = \left[\prod_{i=1}^n \frac{1}{x_i!}\right] \sum \int\int\int p^a (1-p)^b \lambda_1^c \lambda_2^d e^{-f\lambda_1} e^{-g\lambda_2} \frac{1}{\lambda_2^{3/2}}\, dp\, d\lambda_1\, d\lambda_2$$

where a, b, c, d, f and g are all integer constants greater than or equal to 0 and fulfill the conditional relationship (for any $n \geq 1$): if $f = 0 \Rightarrow c = 0$ and $g > 0$; while, if $g = 0 \Rightarrow d = 0$ and $f > 0$. Considering any one term, say R_i, in the summation for R, then

$$R_i = C_1 \int_0^{\infty} \int_0^{\lambda_2} \lambda_1^c \lambda_2^{d-3/2} e^{-f\lambda_1} e^{-g\lambda_2} \int_0^1 p^a (1-p)^b \, dp \, d\lambda_1 \, d\lambda_2$$

where $C_1 = [\prod_{i=1}^n x_i!]^{-1}$. Recognising the form of the beta distribution and integrating with respect to p gives

$$\begin{aligned} R_i &= C_2 \int_0^{\infty} \int_0^{\lambda_2} \lambda_1^c \lambda_2^{d-3/2} e^{-f\lambda_1} e^{-g\lambda_2} \int_0^1 \frac{p^{(a+1)-1}(1-p)^{(b+1)-1}}{B(a+1, b+1)} \, dp \, d\lambda_1 \, d\lambda_2 \\ &= C_2 \int_0^{\infty} \int_0^{\lambda_2} \lambda_1^c \lambda_2^{d-3/2} e^{-f\lambda_1} e^{-g\lambda_2} \, d\lambda_1 \, d\lambda_2 \end{aligned}$$

where $C_2 = C_1 \, B(a+1, b+1)$. We now explore R_i for all variable potentialities.

For $f = 0$

Using the conditional relationship $f = 0 \Rightarrow c = 0$ and $g > 0$, and recognising the form of the gamma distribution, then

$$\begin{aligned} R_i &= C_2 \int_0^{\infty} \lambda_2^{d-3/2} e^{-g\lambda_2} \int_0^{\lambda_2} 1 \, d\lambda_1 \, d\lambda_2 \\ &= C_2 \int_0^{\infty} \lambda_2^{d-1/2} e^{-g\lambda_2} \, d\lambda_2 \\ &= C_2 \frac{\Gamma(d+1/2)}{g^{d+1/2}} \int_0^{\infty} \frac{g^{d+1/2}}{\Gamma(d+1/2)} \lambda_2^{(d+1/2)-1} e^{-g\lambda_2} \, d\lambda_2 \\ &= B(a+1, b+1) \frac{\Gamma(d+1/2)}{g^{d+1/2}} \left[\prod_{i=1}^n \frac{1}{x_i!} \right] \end{aligned}$$

which is defined.

For $g = 0$

Using the conditional relationship $g = 0 \Rightarrow d = 0$ and $f > 0$, reversing the order of integration and recognising the form of the gamma distribution, then

$$R_i = C_2 \int_0^{\infty} \lambda_1^c e^{-f\lambda_1} \int_{\lambda_1}^{\infty} \lambda_2^{-3/2} \, d\lambda_2 \, d\lambda_1$$

$$= 2\,C_2 \int_0^\infty \lambda_1^{c-1/2} e^{-f\lambda_1}\, d\lambda_1$$

$$= 2\,C_2 \frac{\Gamma(c+1/2)}{f^{c+1/2}} \int_0^\infty \frac{f^{c+1/2}}{\Gamma(c+1/2)} \lambda_1^{(c+1/2)-1} e^{-f\lambda_1}\, d\lambda_1$$

$$= 2\,B(a+1,b+1) \frac{\Gamma(c+1/2)}{f^{c+1/2}} \left[\prod_{i=1}^{n} \frac{1}{x_i!}\right]$$

which is defined.

For both $f > 0$ and $g > 0$

Recognising the form of the gamma distribution, R_i can be rewritten as

$$R_i = C_2 \int_0^\infty \lambda_2^{d-3/2} e^{-g\lambda_2} \int_0^{\lambda_2} \lambda_1^c e^{-f\lambda_1}\, d\lambda_1\, d\lambda_2$$

$$= C_2 \int_0^\infty \lambda_2^{d-3/2} e^{-g\lambda_2} \frac{\Gamma(c+1)}{f^{c+1}} \int_0^{\lambda_2} \frac{f^{c+1}}{\Gamma(c+1)} \lambda_1^{(c+1)-1} e^{-f\lambda_1}\, d\lambda_1\, d\lambda_2$$

and noting from Mood, Graybill and Boes (1986), page 114, that

$$\int_0^x \frac{\lambda^r}{\Gamma(r)} u^{r-1} e^{-\lambda u}\, du = 1 - \sum_{j=0}^{r-1} e^{-\lambda x} \frac{(\lambda x)^j}{j!} \tag{4.14}$$

then upon reparameterisation and substitution, the integration becomes

$$R_i = C_3 \int_0^\infty \lambda_2^{d-3/2} e^{-g\lambda_2} \left[1 - \sum_{j=0}^{c} e^{-f\lambda_2} \frac{(f\lambda_2)^j}{j!}\right] d\lambda_2$$

$$= C_3 \int_0^\infty \lambda_2^{d-3/2} e^{-g\lambda_2} \left[1 - e^{-f\lambda_2} - \frac{(f\lambda_2)^1}{1!} e^{-f\lambda_2} - \frac{(f\lambda_2)^2}{2!} e^{-f\lambda_2} - \ldots\right] d\lambda_2$$

$$= C_3 \int_0^\infty \lambda_2^{(d-1/2)-1} e^{-g\lambda_2}\, d\lambda_2 - C_3 \int_0^\infty \lambda_2^{(d-1/2)-1} e^{-(g+f)\lambda_2}\, d\lambda_2 - \tag{4.15}$$

$$C_3 \frac{f^1}{1!} \int_0^\infty \lambda_2^{(d+1/2)-1} e^{-(g+f)\lambda_2}\, d\lambda_2 - C_3 \frac{f^2}{2!} \int_0^\infty \lambda_2^{(d+3/2)-1} e^{-(g+f)\lambda_2}\, d\lambda_2 - \ldots$$

where $C_3 = C_2\,\Gamma(c+1)/f^{c+1}$. For $d \geq 1$ it is evident that each integral term in (4.15) can be recognised as being gamma in form and are thus all defined. However, for $d = 0$, this result is not so transparent. We now examine this specific case.

After assigning $d = 0$ in (4.15), the integrals beyond the second term are clearly recognisable as being distributed in a gamma fashion and are therefore proper. It is the first two integral terms that require further specific consideration. Combining these two terms, ignoring the constant C_3 and integrating by parts yields

$$\begin{aligned}\int_0^\infty \lambda_2^{-3/2}\left[e^{-g\lambda_2} - e^{-(g+f)\lambda_2}\right] d\lambda_2 &= -2\left[\frac{e^{-g\lambda_2} - e^{-(g+f)\lambda_2}}{\sqrt{\lambda_2}}\right]_0^\infty + \\ &\qquad 2\int_0^\infty \lambda_2^{-1/2}\left[-ge^{-g\lambda_2} + (g+f)e^{-(g+f)\lambda_2}\right] d\lambda_2. \end{aligned} \tag{4.16}$$

The second term in (4.16) is, once more, clearly recognisable as being a combination of two proper gamma densities, and so it remains to verify that the first term is bounded away from ∞.

When $\lambda_2 \to \infty$, it is clear that

$$\frac{e^{-g\lambda_2}}{\sqrt{\lambda_2}} \to 0 \quad \text{and} \quad \frac{e^{-(g+f)\lambda_2}}{\sqrt{\lambda_2}} \to 0$$

so, in this limit, the first term of (4.16) equals zero. As $\lambda_2 \to 0$, it is useful to expand the exponential terms, viz

$$e^x = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \ldots,$$

to explicitly understand what happens in this limit. Upon expansion,

$$\begin{aligned}\frac{e^{-g\lambda_2}}{\sqrt{\lambda_2}} - \frac{e^{-(g+f)\lambda_2}}{\sqrt{\lambda_2}} &= \left[\frac{1}{\sqrt{\lambda_2}} - g\lambda_2^{1/2} + \frac{g^2}{2!}\lambda_2^{3/2} - \frac{g^3}{3!}\lambda_2^{5/2} + \ldots\right] - \\ &\qquad \left[\frac{1}{\sqrt{\lambda_2}} - (g+f)\lambda_2^{1/2} + \frac{(g+f)^2}{2!}\lambda_{3/2} - \frac{(g+f)^3}{3!}\lambda_2^{5/2} + \ldots\right] \\ &= \left[f\lambda_2^{1/2} + \frac{g^2 - (g+f)^2}{2!}\lambda_2^{3/2} - \frac{g^3 - (g+f)^3}{3!}\lambda_2^{5/2} + \ldots\right]_{\lambda_2 \to 0} \\ &= 0.\end{aligned}$$

This implies that when $d = 0$, the first term of (4.16) is 0 while the second term is some defined value from a gamma density. Summing over R_i ensures that R is bounded away from 0 and ∞ and thus $\pi_3(\boldsymbol{\theta}_3 \mid \boldsymbol{x})$ is proper for $x_i \geq 0$ and $n \geq 1$.

Posterior distribution: $\pi_4(\boldsymbol{\theta}_4 \mid \boldsymbol{x})$

Lastly, the posterior for the geometric density can be derived and written in closed form, as follows. The marginal distribution of $\boldsymbol{x}$ for M_4 is given by

$$\begin{aligned}\int f_4(\boldsymbol{x} \mid \boldsymbol{\theta}_4)\, \pi_4(\boldsymbol{\theta}_4)\, d\boldsymbol{\theta}_4 &= \int_0^1 \left[\prod_{i=1}^{n} p(1-p)^{x_i}\right] \frac{1}{p\sqrt{1-p}} dp \\ &= \int_0^1 p^{n-1}(1-p)^{S-1/2} dp.\end{aligned}$$

Recognising the form of the beta distribution, providing $n > 0$ and $S + 1/2 > 0$, and rewriting the expression gives

$$B(S+1/2, n) \int_0^1 \frac{p^{n-1}(1-p)^{(S+1/2)-1}}{B(S+1/2, n)} dp,$$

which integrates to

$$B(S+1/2, n)$$

so that

$$\pi_4(\boldsymbol{\theta}_4 \mid \boldsymbol{x}) = \frac{p^{n-1}(1-p)^{(S+1/2)-1}}{B(S+1/2, n)}. \tag{4.17}$$

This posterior distribution is clearly recognisable as being beta in distribution and is proper for all $x_i \geq 0$ and $n \geq 1$.

4.5.2 Hold-out predictive distributions

The primary goal of hold-out prediction is to assess how well those observations which are singly omitted from the observed phenomena are forecasted by the predictive model conditioned on the remaining data. Clearly, such techniques are only applicable for $n \geq 2$.

Similar to the posterior distributions derived in the preceding section, the cross-validatory hold-out predictive distributions for M_1 and M_4 can be expressed in closed form while densities M_2 and M_3 require numerical integration.

Predictive distribution: $f_1(x_i \mid \boldsymbol{x}_{(i)})$

It is evident from (4.11) that the M_1 hold-out posterior density is given by

$$\pi_1(\boldsymbol{\theta}_1 \mid \boldsymbol{x}_{(i)}) = \frac{(n-1)^{S_{(i)}+1/2}}{\Gamma(S_{(i)}+1/2)} \lambda^{(S_{(i)}+1/2)-1} e^{-(n-1)\lambda}$$

where $S_{(i)} = \sum_{j=1,j\neq i}^{n} x_j$. From (4.4) it is apparent that the hold-out predictive can be derived by noting

$$\begin{aligned} f_1(x_i \mid \boldsymbol{x}) &= \int_0^\infty \frac{\lambda^{x_i} e^{-\lambda}}{x_i!} \frac{(n-1)^{S_{(i)}+1/2}}{\Gamma(S_{(i)}+1/2)} \lambda^{(S_{(i)}+1/2)-1} e^{-(n-1)\lambda} d\lambda \\ &= \frac{(n-1)^{S_{(i)}+1/2}}{x_i!\,\Gamma(S_{(i)}+1/2)} \int_0^\infty \lambda^{(S_{(i)}+x_i+1/2)-1} e^{-n\lambda} d\lambda. \end{aligned}$$

Recognising the gamma distribution, providing $S_{(i)} + x_i + 1/2 > 0$ and $n > 0$, this expression can be rewritten as

$$\frac{(n-1)^{S_{(i)}+1/2}\,\Gamma(S_{(i)}+x_i+1/2)}{x_i!\,\Gamma(S_{(i)}+1/2)\,n^{S_{(i)}+x_i+1/2}} \int_0^\infty \frac{n^{S_{(i)}+x_i+1/2}}{\Gamma(S_{(i)}+x_i+1/2)} \lambda^{(S_{(i)}+x_i+1/2)-1} e^{-n\lambda} d\lambda$$

and upon integration equals

$$\begin{aligned} f_1(x_i \mid \boldsymbol{x}_{(i)}) &= \frac{(n-1)^{S_{(i)}+1/2}\,\Gamma(S_{(i)}+x_i+1/2)}{x_i!\,\Gamma(S_{(i)}+1/2)\,n^{S_{(i)}+x_i+1/2}} \\ &= \binom{S_{(i)}+x_i-1/2}{x_i} \left(1-\frac{1}{n}\right)^{S_{(i)}+1/2} \left(\frac{1}{n}\right)^{x_i}, \end{aligned} \tag{4.18}$$

which is negative binomial in distribution. This hold-out predictive density is, therefore, proper providing $x_i \geq 0$ and $S_{(i)} \geq 0$ for any $n \geq 2$. Exploiting the negative binomial form, it is straightforward to derive

$$\begin{aligned} \mu_{1(i)} &= \mathrm{E}_1[X_i \mid \boldsymbol{x}_{(i)}] = \frac{S_{(i)}+1/2}{n-1} \quad \text{and} \\ \sigma^2_{1(i)} &= Var_1(X_i \mid \boldsymbol{x}_{(i)}) = \frac{n\,(S_{(i)}+1/2)}{(n-1)^2}. \end{aligned} \tag{4.19}$$

Predictive distribution: $f_2(x_i \mid \boldsymbol{x}_{(i)})$

From (4.12), it is clear that computation of $\pi_2(\boldsymbol{\theta}_2 \mid \boldsymbol{x}_{(i)})$ requires one-dimensional numerical integration over a with

$$\pi_2(\boldsymbol{\theta}_2 \mid \boldsymbol{x}_{(i)}) = \frac{1}{R} \left[\prod_{j=1,j\neq i}^{n} \binom{x_j+a-1}{x_j} \right] \frac{p^{(n-1)a}(1-p)^{S_{(i)}}}{\sqrt{a+1}}\, da$$

where

$$R = \int_0^\infty \left[\prod_{j=1,j\neq i}^{n} \binom{x_j+a-1}{x_j} \right] \frac{B(S_{(i)}+1,(n-1)a+1)}{\sqrt{a+1}}\, da.$$

Hence, this hold-out predictive density has the form

$$f_2(x_i \mid \boldsymbol{x}_{(i)}) = \tag{4.20}$$
$$\frac{1}{R}\int_0^\infty \binom{x_i+a-1}{x_i}\left[\prod_{j=1,j\neq i}^{n}\binom{x_j+a-1}{x_j}\right]\frac{B(S_{(i)}+x_i+1,na+1)}{\sqrt{a+1}}\,da$$

which is proper for $S_i > 0$ and $n \geq 2$.

Recalling (2.4), then the mean for this hold-out predictive density can be found by noting

$$\begin{aligned}
\mu_{2(i)} &= \mathrm{E}_2[X_i \mid \boldsymbol{x}_{(i)}] \\
&= \int\left[\sum_{i=0}^{\infty} x_i f_2(x_i \mid \boldsymbol{\theta}_2)\right]\pi_2(\boldsymbol{\theta}_2 \mid \boldsymbol{x}_{(i)})\,d\boldsymbol{\theta}_2 \\
&= \frac{1}{R}\int_0^1\int_0^\infty \frac{a(1-p)}{p}\left[\prod_{j=1,j\neq i}^{n}\binom{x_j+a-1}{x_j}\right]\frac{p^{(n-1)a}(1-p)^{S_{(i)}}}{\sqrt{a+1}}\,da\,dp \\
&= \frac{1}{R}\int_0^\infty\left[\prod_{j=1,j\neq i}^{n}\binom{x_j+a-1}{x_j}\right]B(S_{(i)}+2,(n-1)a)\frac{a}{\sqrt{a+1}}\times \\
&\quad \int_0^1 \frac{p^{(n-1)a-1}(1-p)^{(S_{(i)}+2)-1}}{B(S_{(i)}+2,(n-1)a)}\,dp\,da. \\
&= \frac{1}{R}\int_0^\infty\left[\prod_{j=1,j\neq i}^{n}\binom{x_j+a-1}{x_j}\right]B(S_{(i)}+2,(n-1)a)\,\frac{a}{\sqrt{a+1}}\,da
\end{aligned}$$

since the parameters in the beta distribution for the integral over p are both positive. Using a similar strategy to that described in the previous section, it is straightforward to show that this mean is defined for $n \geq 2$.

Unfortunately, this property does not hold for the variance. Noting from (2.4) that

$$\mathrm{E}_2[X_i^2 \mid \boldsymbol{x}_{(i)}] = \frac{a(1-p)}{p^2} + \frac{a^2(1-p)^2}{p^2},$$

then the second moment for this hold-out predictive density can be expressed by

$$\mathrm{E}_2[X_i^2 \mid \boldsymbol{x}_{(i)}] =$$
$$\frac{1}{R}\int_0^\infty\left[\prod_{j=1,j\neq i}^{n}\binom{x_j+a-1}{x_j}\right]B(S_{(i)}+2,a(n-1)-1)\,\frac{a}{\sqrt{a+1}}\,da \quad +$$

$$\frac{1}{R}\int_0^\infty \left[\prod_{j=1,j\neq i}^{n}\binom{x_j+a-1}{x_j}\right] B(S_{(i)}+3, a(n-1)-1)\,\frac{a^2}{\sqrt{a+1}}\,da \tag{4.21}$$

and this does not exist for $a \leq 1/(n-1)$. Consequently, this implies $\sigma^2_{2(i)}$ does not exist for $a \leq 1/(n-1)$.

Predictive distribution: $f_3(x_i \mid \boldsymbol{x}_{(i)})$

It is evident that the hold-out predictive distribution for the mixture of two Poisson distributions can be expressed by

$$f_3(x_i \mid \boldsymbol{x}_{(i)}) = \tag{4.22}$$
$$\frac{\int\int\int \left(\frac{p\lambda_1^{x_i}e^{-\lambda_1}}{x_i!}+\frac{q\lambda_2^{x_i}e^{-\lambda_2}}{x_i!}\right)\left[\prod_{j=1,i\neq j}^{n}\frac{p\lambda_1^{x_j}e^{-\lambda_1}}{x_j!}+\frac{q\lambda_2^{x_j}e^{-\lambda_2}}{x_j!}\right]\frac{1}{\lambda_2^{3/2}}\,dp\,d\lambda_1\,d\lambda_2}{\int\int\int \left[\prod_{j=1,i\neq j}^{n}\frac{p\lambda_1^{x_j}e^{-\lambda_1}}{x_j!}+\frac{q\lambda_2^{x_j}e^{-\lambda_2}}{x_j!}\right]\frac{1}{\lambda_2^{3/2}}\,dp\,d\lambda_1\,d\lambda_2}$$

where $q = 1-p$. Additionally, using the results presented for (4.13), which are paralleled here, it is clear that both the numerator and denominator of (4.22) are proper for all $x_i \geq 0$ and $n \geq 2$.

Recalling from (2.6) that the mean of a mixture of two Poisson distributions is $\mathrm{E}_3[X_i] = p\lambda_1 + (1-p)\lambda_2$, then this predictive distribution has mean given by

$$\begin{aligned}
\mu_{3(i)} &= \mathrm{E}_3[X_i \mid \boldsymbol{x}_{(i)}] \\
&= \int\left[\sum_{i=0}^{\infty} x_i f_3(x_i \mid \boldsymbol{\theta}_3)\right]\pi_3(\boldsymbol{\theta}_3 \mid \boldsymbol{x}_{(i)})\,d\boldsymbol{\theta}_3 \\
&= \frac{\int\int\int [p\lambda_1+(1-p)\lambda_2]\left[\prod_{j=1,i\neq j}^{n}\frac{p\lambda_1^{x_j}e^{-\lambda_1}}{x_j!}+\frac{q\lambda_2^{x_j}e^{-\lambda_2}}{x_j!}\right]\frac{1}{\lambda_2^{3/2}}\,dp\,d\lambda_1\,d\lambda_2}{\int\int\int \left[\prod_{j=1,i\neq j}^{n}\frac{p\lambda_1^{x_j}e^{-\lambda_1}}{x_j!}+\frac{q\lambda_2^{x_j}e^{-\lambda_2}}{x_j!}\right]\frac{1}{\lambda_2^{3/2}}\,dp\,d\lambda_1\,d\lambda_2}.
\end{aligned}$$

To verify whether this expression yields a defined mean only the numerator requires specific consideration as, from above, it is clear that the denominator is always defined and bounded away from 0 and ∞ for $x_i \geq 0$ and $n \geq 2$. After expansion, the numerator has one term that takes the form

$$\int\int\int (1-p)\lambda_2\left[\prod_{j=1,j\neq i}^{n}\frac{p\lambda_1^{x_j}e^{-\lambda_1}}{x_j!}\right]\frac{1}{\lambda_2^{3/2}}\,dp\,d\lambda_1\,d\lambda_2$$

which can be integrated with respect to p so that

$$\left[\prod_{j=1,j\neq i}^{n}\frac{1}{x_j!}\right]\int\int\frac{\lambda_1^{S_{(i)}}e^{-(n-1)\lambda_1}}{\sqrt{\lambda_2}}\int_0^1(1-p)p^{n-1}dp\,d\lambda_1\,d\lambda_2 =$$

$$C_1\int\int\frac{\lambda_1^{S_{(i)}}e^{-(n-1)\lambda_1}}{\sqrt{\lambda_2}}\,d\lambda_1\,d\lambda_2$$

where $C_1 = \left[n(n+1)\prod_{j=1,j\neq i}^{n}x_j!\right]^{-1}$. Integrating with respect to λ_1 and recalling (4.14) then

$$\begin{aligned}
&C_1\int_0^\infty\int_0^{\lambda_2}\frac{\lambda_1^{S_{(i)}}e^{-(n-1)\lambda_1}}{\sqrt{\lambda_2}}\,d\lambda_1\,d\lambda_2\\
&= C_1\int_0^\infty\frac{1}{\sqrt{\lambda_2}}\frac{\Gamma(S_{(i)}+1)}{(n-1)^{S_{(i)}+1}}\int_0^{\lambda_2}\frac{(n-1)^{S_{(i)}+1}}{\Gamma(S_{(i)}+1)}\lambda_1^{(S_{(i)}+1)-1}e^{-(n-1)\lambda_1}\,d\lambda_1\,d\lambda_2\\
&= C_2\int_0^\infty\frac{1}{\sqrt{\lambda_2}}\left[1-\sum_{j=0}^{S_{(i)}}\frac{[(n-1)\lambda_2]^j}{j!}e^{-(n-1)\lambda_2}\right]d\lambda_2\\
&= C_2\int_0^\infty\frac{1}{\sqrt{\lambda_2}}\,d\lambda_2 - C_2\int_0^\infty\lambda_2^{(1/2)-1}e^{-(n-1)\lambda_2}\,d\lambda_2 -\\
&\quad C_2\,(n-1)\int_0^\infty\lambda_2^{(3/2)-1}e^{-(n-1)\lambda_2}\,d\lambda_2 - \ldots
\end{aligned}$$

where $C_2 = C_1\Gamma(S_{(i)}+1)/(n-1)^{S_{(i)}+1}$. Integral terms beyond the first are all clearly recognisable as being distributed in a gamma fashion and thus are bounded. The difficulty stems from the first integral term

$$C_2\int_0^\infty\frac{1}{\sqrt{\lambda_2}}\,d\lambda_2 = 2C_2\left[\sqrt{\lambda_2}\right]_0^\infty\to\infty.$$

This implies that the mean of (4.22) does not exist. Moreover, because $\mathrm{E}_3[X_i \mid \boldsymbol{x}_{(i)}]$ does not exist, then $\mathrm{E}_3[X_i^2 \mid \boldsymbol{x}_{(i)}]$ also does not exist and so the variance of (4.22) is not defined.

Predictive distribution: $f_4(x_i \mid \boldsymbol{x}_{(i)})$

From (4.17), it is clear that the hold-out posterior distribution for M_4 has the form

$$\pi_4(\theta_4 \mid \boldsymbol{x}_{(i)}) = \frac{p^{(n-1)-1}(1-p)^{(S_{(i)}+1/2)-1}}{B(S_{(i)}+1/2, n-1)}$$

which is proper for all $x_i \geq 0$ and $n \geq 2$. Now the hold-out predictive density is given by

$$\begin{aligned} f_4(x_i \mid \boldsymbol{x}_{(i)}) &= \int_0^1 p(1-p)^{x_i} \frac{p^{(n-1)-1}(1-p)^{(S_{(i)}+1/2)-1}}{B(S_{(i)}+1/2, n-1)}\, dp \\ &= \frac{B(S_{(i)}+x_i+1/2, n)}{B(S_{(i)}+1/2, n-1)} \int_0^1 \frac{p^{(n)-1}(1-p)^{(S_{(i)}+x_i+1/2)-1}}{B(S_{(i)}+x_i+1/2, n)}\, dp \\ &= (n-1)\, \frac{\Gamma(S_{(i)}+x_i+1/2)\, \Gamma(S_{(i)}+n-1/2)}{\Gamma(S_{(i)}+1/2)\, \Gamma(S_{(i)}+x_i+n+1/2)}, \end{aligned} \tag{4.23}$$

after recognising the beta distribution.

Noting from (2.8) that the mean of a geometric distribution is $\mathrm{E}_4[X_i] = (1-p)/p$ and adopting standard statistical principles, this hold-out predictive distribution has mean given by

$$\begin{aligned} \mu_{4(i)} &= \mathrm{E}_4[X_i \mid \boldsymbol{x}_{(i)}] \\ &= \int \left[\sum_{i=0}^{\infty} x_i f_4(x_i \mid \boldsymbol{\theta}_4)\right] \pi_4(\boldsymbol{\theta}_4 \mid \boldsymbol{x}_{(i)})\, d\boldsymbol{\theta}_4 \\ &= \int_0^1 \frac{(1-p)}{p} \frac{p^{(n-1)-1}(1-p)^{(S_{(i)}+1/2)-1}}{B(S_{(i)}+1/2, n-1)}\, dp \\ &= \frac{B(S_{(i)}+3/2, n-2)}{B(S_{(i)}+1/2, n-1)} \int_0^1 \frac{p^{(n-2)-1}(1-p)^{(S_{(i)}+3/2)-1}}{B(S_{(i)}+3/2, n-2)}\, dp \\ &= \frac{S_{(i)}+1/2}{n-2} \end{aligned}$$

which is proper providing $n \geq 3$.

It is clear from (2.8) that the second moment of a geometric distribution is $\mathrm{E}_4[X_i^2] = (1-p)(2-p)/p^2$ and so the corresponding second moment of the hold-out predictive distribution takes the form

$$\begin{aligned} \mathrm{E}_4[x_i^2 \mid \boldsymbol{x}_{(i)}] &= \int \left[\sum_{i=0}^{\infty} x_i^2 f_4(x_i \mid \boldsymbol{\theta}_4)\right] \pi_4(\boldsymbol{\theta}_4 \mid \boldsymbol{x}_{(i)})\, d\boldsymbol{\theta}_4 \\ &= \int_0^1 \frac{(1-p)(2-p)}{p^2} \frac{p^{(n-1)-1}(1-p)^{(S_{(i)}+1/2)-1}}{B(S_{(i)}+1/2, n-1)}\, dp \end{aligned}$$

$$= 2\int_0^1 \frac{(1-p)}{p^2}\frac{p^{(n-1)-1}(1-p)^{(S_{(i)}+1/2)-1}}{B(S_{(i)}+1/2,n-1)}\,dp - \qquad \text{(term 1)}$$

$$\int_0^1 \frac{(1-p)}{p}\frac{p^{(n-1)-1}(1-p)^{(S_{(i)}+1/2)-1}}{B(S_{(i)}+1/2,n-1)}\,dp. \qquad \text{(term 2)}$$

Studying term 1, recognising the beta density,

$$\text{term 1} = 2\frac{B(S_{(i)}+3/2,n-3)}{B(S_{(i)}+1/2,n-1)}\int_0^1 \frac{p^{(n-3)-1}(1-p)^{(S_{(i)}+3/2)-1}}{B(S_{(i)}+3/2,n-3)}\,dp$$

$$= 2\frac{(S_{(i)}+1/2)\,(S_{(i)}+n-3/2)}{(n-2)\,(n-3)}$$

providing $n \geq 4$. Noting that term 2 is simply $\mu_{4(i)}$, then

$$\mathrm{E}_4[x_i^2 \mid \boldsymbol{x}_{(i)}] = 2\frac{(S_{(i)}+1/2)\,(S_{(i)}+n-3/2)}{(n-2)\,(n-3)} - \frac{S_{(i)}+1/2}{n-2}$$

$$= \frac{(S_{(i)}+1/2)\,(2S_{(i)}+n)}{(n-2)\,(n-3)}$$

and therefore

$$\sigma^2_{4(i)} = \mathrm{E}_4[x_i^2 \mid \boldsymbol{x}_{(i)}] - \left(\mathrm{E}_4[x_i \mid \boldsymbol{x}_{(i)}]\right)^2$$

$$= \frac{(S_{(i)}+1/2)\,(2S_{(i)}+n)}{(n-2)\,(n-3)} - \left(\frac{S_{(i)}+1/2}{n-2}\right)^2$$

$$= \frac{(n-1)(S_{(i)}+1/2)(S_{(i)}+n-3/2)}{(n-2)^2(n-3)}$$

providing $n \geq 4$.

4.5.3 Computational methods

When the distributions $\pi_j(\boldsymbol{\theta}_j \mid \boldsymbol{x})$ and $f_j(x_i \mid \boldsymbol{x}_{(i)})$ are available in closed form, then generation of the $\widehat{\mathcal{F}}^r(d \mid j,j)$ and $\widehat{\mathcal{F}}^r(d \mid j,k)$ distributions can easily be achieved. A package that facilitates large matrix computations (such as MATLAB) is suitable for this type of generation process. For $N = 10,000$ and using a SUN Sparc 10 computer, it took approximately 5–10 minutes to perform the generations used in Section 4.6, depending on the sample size n. Calculated estimates were within $\pm 0.5\%$, found from repeated computation of the same problem.

When neither $\pi_j(\boldsymbol{\theta}_j \mid \boldsymbol{x})$ nor $f_j(x_i \mid \boldsymbol{x}_{(i)})$ are available in closed form, then numerical approximations are necessary. While conceptually the process of obtaining the adequacy distributions remains straightforward, the disadvantage is that considerably more computer resources are required. Specifically, the difficulty arises when multiple determinations of $f_j(x_i \mid \boldsymbol{x}_{(i)})$, $\mu_{j(i)}$ and $\sigma^2_{j(i)}$ are required over i for each of the N generated samples. It might be tempting to approximate the hold-out predictive density function by $f_j(x_i \mid \boldsymbol{x})$, reducing the numerical integral evaluations. However, Gelfand, Dey and Chang (1992) claim that this should be avoided, as $f_j(x_i \mid \boldsymbol{x})$ may be quite different from $f_j(x_i \mid \boldsymbol{x}_{(i)})$, even when x_i's are assumed to be conditionally independent.

In this thesis, acquisition of $\boldsymbol{\theta}_j^i$ values from $\pi_j(\boldsymbol{\theta}_j \mid \boldsymbol{x})$ was easily made using the sample-resample method of Smith and Gelfand (1992). For the determination of integrals relating to $f_2(x_i \mid \boldsymbol{x}_{(i)})$, the trapezoidal rule was readily and accurately applied, while the sample-mean Monte Carlo method (Rubinstein, 1981) was adopted to approximate $f_3(x_i \mid \boldsymbol{x}_{(i)})$, $\mu_{3(i)}$, $\sigma^2_{3(i)}$ and related integrations. This sample-mean Monte Carlo integration technique allows an approximation to the desired 3–dimensional integrals to be computed within a feasible time frame, provided a facility exists where large matrix manipulations can easily be handled (such as in MATLAB). The parameter space bound used when adopting the sample-mean Monte Carlo method was $0 < \lambda_1 < \lambda_2 < 100$. In the accident analysis context, it is considered unlikely that driver factors or vehicle and environmental factors would have an annual underlying accident rate exceeding ten, so it could be construed that the upper bound of 100 on the λ_2 parameter space is conservative.

Simulations of size $N = 2,500$ were used when these integral approximation methods were employed in Section 4.6. Computations occupied a SUN Sparc 10 computer for approximately 1–3 hours, depending on the sample size n. Calculated estimates were almost invariably within $\pm 2\%$, again found from repeated calculation of the same problem.

4.5.4 Mean and variance adjustments

From the mathematical details provided in Section 4.5.2, it was evident that the hold-out predictive distribution $f_3(x_i \mid \boldsymbol{x}_{(i)})$ has mean and variance that tends to infinity for unbounded λ_2 while $f_2(x_i \mid \boldsymbol{x}_{(i)})$ has an undefined variance when $a \leq$

$1/(n-1)$. Strictly speaking, this implies that both the M_2 and M_3 models can not have their adequacy checked using the $\mathcal{D}^1$ measure. However, it is also apparent that in using the proposed simulation scheme, in conjunction with the aforementioned trapezoidal and MCMC integration techniques, defined *pseudo-mean* and *pseudo-variance* values can be estimated.

For the numerical calculations involving the M_2 model, a *pseudo-variance* was determined by constraining $a > 1/(n-1)$. Similarly, because numerical approximations for M_3 used a bounded space $0 < \lambda_1 < \lambda_2 < 100$, both *pseudo-mean* and *pseudo-variance* values exist and were estimated for this model. Once ascertained, these values were then used to derive adequacy measures associated with $\mathcal{D}^1(M_2)$ and $\mathcal{D}^1(M_3)$, respectively.

It should be noted that these *pseudo-values* depend on the restricting the allowable parameter space. This dependency suggests that different model adequacy conclusions may be drawn from different boundary specification, although this has yet to be fully confirmed. The usefulness of adopting such *pseudo-values* in the determination of $\mathcal{D}^1$ measures is investigated in the ensuing numerical example.

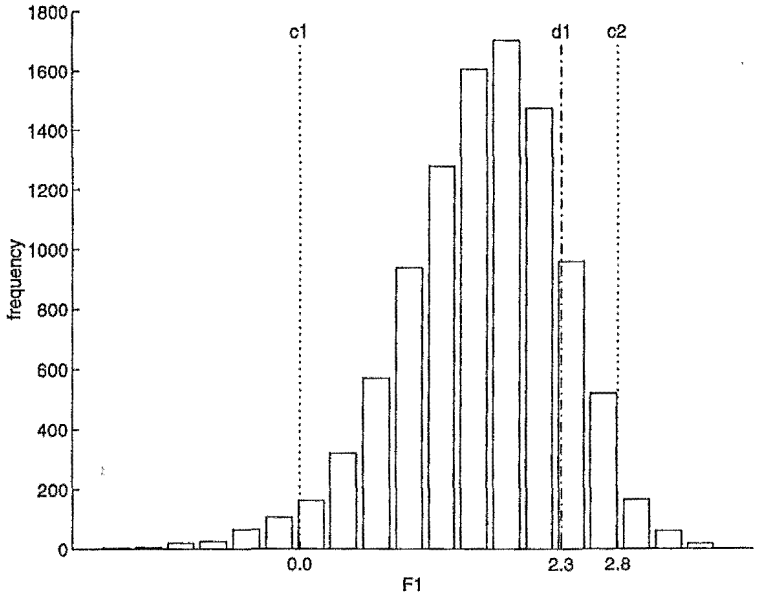
4.6 Numerical results

4.6.1 Adequacy of models

Adopting the simulation approach detailed in Section 4.4, using the computational methods of above, we can now examine the adequacy of each of the four candidate distributions. Figure 4.1 illustrates results typically yielded from one such simulation.

From Figure 4.1 notice that of the $\log D_i^1(M_1, M_1)$ values generated, 95% lie within the (0.0, 2.8) interval while 2.5% fall below 0.0 and 2.5% record values above 2.8. Consistent with traditional statistical logic, values outside this interval, for a two-sided rejection region, are deemed unlikely at $\alpha = 0.05$ under the assumed Poisson model. This implies that the critical values should be assigned $\log \widehat{c}^1_{0.025}(M_1) = 0.0$ and $\log \widehat{c}^1_{0.975}(M_1) = 2.8$, thereby specifying the bounds for the rejection region of this model's adequacy. Should the observed adequacy measurement, $\log d^1(M_1)$, lie outside the (0.0, 2.8) interval, then we would classify M_1 model

Figure 4.1: Histogram of the $\log D_i^1(M_1, M_1)$ adequacy measurement values evaluated for Site 1 from a simulation of size $N = 10,000$. The symbols d1 and F1 are used to denote the $\log d^1(M_1)$ value and the $\log \widehat{\mathcal{F}}^1(d \mid 1,1)$ distribution, respectively, while c1 and c2 give the corresponding critical values at $\alpha = 0.05$.



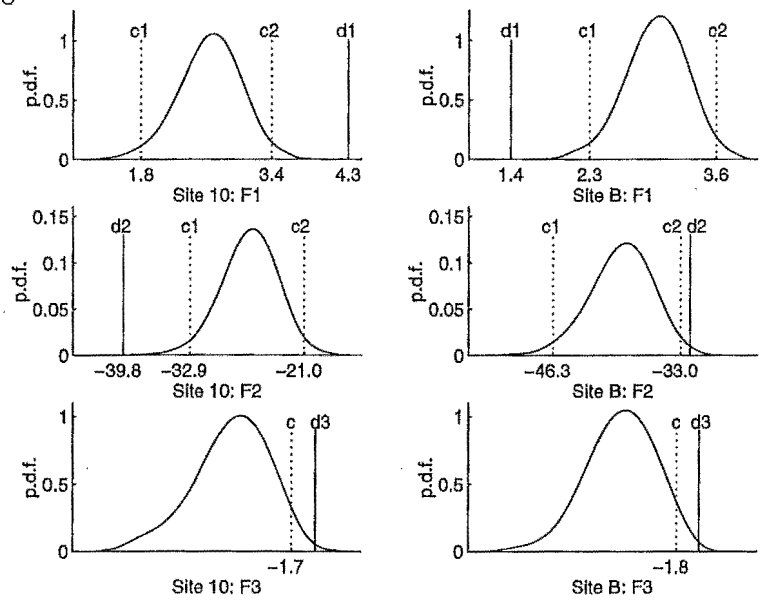
as being inadequate in describing the data at $\alpha = 0.05$.

For the specific example presented in Figure 4.1, which investigates Poison adequacy at Site 1, the observed adequacy measurement $\log d^1(M_1) = 2.3$, a value contained within the (0.0, 2.8) interval. This $\log d^1(M_1)$ value is consistent with the estimated $\log \widehat{\mathcal{F}}^1(d \mid 1,1)$ distribution under M_1, and so it can be concluded that if M_1 had been selected at Site 1, there would be no evidence to dispute its adequacy.

Consider now Figure 4.2 which depicts the results of the three examined adequacy measures at Sites 10 and B under the Poisson assumption. The left hand side graphics illustrate the $\log \widehat{\mathcal{F}}^1(d \mid 1,1)$, $\log \widehat{\mathcal{F}}^2(d \mid 1,1)$ and $\log \widehat{\mathcal{F}}^3(d \mid 1,1)$ distributions associated with Site 10, while the right hand side graphics give the corresponding distributions for the Site B data (although the origin of Site B's data is known, we treat it as unknown).

The empirical dispersion index (estimated variance to mean ratio) for Site 10 is 4.08, so the data appear considerably more dispersed than could be expected under the Poisson assumption. This intuition is confirmed by each of the adequacy measures used. For $\mathcal{D}^1$ adequacy, the observed $\log d^1(M_1)$ measure lies to the right of its expected distribution of $\log \widehat{\mathcal{F}}^1(d \mid 1,1)$ measures if the data were truly Poisson

Figure 4.2: Distributions of the three adequacy measures under the Poisson model at Sites 10 and B, computed from simulations of size $N = 10,000$. The symbols dr and Fr are used to denote $\log d^r(M_1)$ values and $\log \widehat{\mathcal{F}}^r(d \mid 1,1)$ distributions, respectively, while c, c1 and c2 give the corresponding critical values at $\alpha = 0.05$.



distributed. Similarly, $\log d^2(M_1)$ lies to the left and $\log d^3(M_1)$ to the right of their associated expected distributions under the Poisson assumption. Using any of these measures, we would deem M_1 (Poisson) as being inadequate at describing Site 10 data at $\alpha = 0.05$.

Site B recorded an empirical dispersion index of 0.21 which, in this instance, suggested that the data were more under-dispersed than anticipated from the Poisson assumption. This suggestion is substantiated by each of the three adequacy measures rejecting the Poisson assumption at $\alpha = 0.05$. For this scenario, $\log d^1(M_1)$ and $\log d^2(M_1)$ values lie on the opposite side of their associated expected distributions to that when Site 10 was investigated, while $\log d^3(M_1)$ again lies to the right. This diagrammatically verifies the two-sided nature of the $\mathcal{D}^1$ and $\mathcal{D}^2$ adequacy measure test and the one-sided nature of $\mathcal{D}^3$.

Tables C.1–C.4 included in Appendix C summarise the adequacy analyses undertaken on each of the four candidate models at the 35 accident sites using adequacy measures $\mathcal{D}^r$, $r = 1,2,3$. In practice, it is envisaged that only those models generally discriminated as *best*, and thus with the potential of being selected, will have their adequacy checked. However, for the purpose of illustration and investigation

we include adequacy computations for all four models. Additionally presented in Tables C.1–C.4 is the relative *rank* of each candidate model at each site, determined using the previously reported averaged Bayes factor calculations.

Recall that the hold-out predictive distributions $f_2(x_i \mid \boldsymbol{x}_{(i)})$ and $f_3(x_i \mid \boldsymbol{x}_{(i)})$ have undefined mean and variance quantities and *pseudo-entities* were used. Results from the application of these *pseudo-entities* appear in columns 3 and 4 of both Tables C.2 and C.3.

The model adequacy results included in Tables C.1–C.4 are now summarised in Table 4.1. This table lists the number of instances model inadequacy was identified, as determined by the $\mathcal{D}^1$, $\mathcal{D}^2$ and $\mathcal{D}^3$ measures at $\alpha = 0.05$, for each of the four candidate models. Moreover, these lists have been stratified by the averaged Bayes factor discrimination rank recorded by these models over the 35 accident sites.

Table 4.1: Frequency of model *inadequacy* ($\alpha = 0.05$) at the 35 sites using three $\mathcal{D}^r$ measures stratified by the model's discrimination rank (established using the averaged Bayes factor).

Poisson				
Rank	sites	$\mathcal{D}^1$	$\mathcal{D}^2$	$\mathcal{D}^3$
1	22	1	0	0
2	4	0	0	0
3	2	1	0	0
4	7	6	1	4
Total	35	8	1	4

Poisson/gamma				
Rank	sites	$\mathcal{D}^1$	$\mathcal{D}^2$	$\mathcal{D}^3$
1	7	0	0	1
2	28	2	0	1
3	0	0	0	0
4	0	0	0	0
Total	35	2	0	2

mixture of 2 Poissons				
Rank	sites	$\mathcal{D}^1$	$\mathcal{D}^2$	$\mathcal{D}^3$
1	0	0	0	0
2	2	0	0	0
3	31	1	0	1
4	2	0	0	0
Total	35	1	0	1

geometric				
Rank	sites	$\mathcal{D}^1$	$\mathcal{D}^2$	$\mathcal{D}^3$
1	6	0	0	0
2	1	0	0	0
3	2	0	0	0
4	26	13	0	14
Total	35	13	0	14

The adequacy measures

Examination of Table 4.1 reveals that, in terms of absolute numbers, the $\mathcal{D}^1$ measure was the most proficient in identifying model inadequacy of the three measures considered. This measure detected model inadequacy on 24 occasions while the $\mathcal{D}^2$ and

$\mathcal{D}^3$ identified inadequacy in one and 21 instances, respectively. However, aside from Poisson model adequacy considerations, the $\mathcal{D}^3$ measure was seen to identify model inadequacy with a similar degree of proficiency as that demonstrated by the $\mathcal{D}^1$ measure. By comparison, the $\mathcal{D}^2$ measure discerned model inadequacy infrequently and with the least success.

This phenomenon featured most prominently in Table 4.1 when geometric adequacy was considered. While both the $\mathcal{D}^1$ and $\mathcal{D}^3$ measures consistently rejected the adequacy of the geometric model (in 37% and 40%, respectively, of the 35 instances considered), the $\mathcal{D}^2$ adequacy measure was unable to demonstrate once that this model was incompatible with the data. This result can be explained by a deficiency inherent in this measure, as a measure of goodness-of-fit, for this type of data; further explanation will follow in Section 4.6.3.

The consistency between adequacy measures in determining model inadequacy can be assessed by referring to Tables C.1–C.4. It is evident from perusal of these tables that the instance where model inadequacy was identified by the $\mathcal{D}^2$ measure, both the $\mathcal{D}^1$ and $\mathcal{D}^3$ measures also demonstrated inadequacy. Moreover, model inadequacy was identified by the $\mathcal{D}^3$ measure on 21 occasions, and of these 17 (81%) were also identified by the $\mathcal{D}^1$ measure.

These results demonstrated that model inadequacy was identified with some degree of consistency between the three examined adequacy measures, particularly between the $\mathcal{D}^1$ and $\mathcal{D}^3$ measures. However, as these measures investigate different characteristics of the assumed model, some differences in the identification of model inadequacy naturally existed.

Model performance

A distinguishing feature of Table 4.1 was the relatively high number of sites at which the Poisson model was found to be inadequate. Based upon the $\mathcal{D}^1$ adequacy measurement calculations, model inconsistency with the empirical data was demonstrated at eight (23%) sites. Identification of Poisson inadequacy was not as frequent with the adoption of the $\mathcal{D}^2$ and $\mathcal{D}^3$ measures; with one (3%) and four sites (11%), respectively, meeting the rejection criterion.

Another noteworthy feature of this investigation was the identification of M_1 model inadequacy by the $\mathcal{D}^1$ measure at Site 6, a site where the Poisson model had

previously been discriminated as being the best model. Examination of the data at Site 6 revealed a high degree of under-dispersion, with the estimated dispersion index equalling 0.453. Not surprisingly, none of the considered candidate models were adjudged as adequately describing this under-dispersed data by this measure.

Sites modelled by the Poisson/gamma model were identified as being inadequate in only two (6%) instances by both the $\mathcal{D}^1$ and $\mathcal{D}^3$ measures. The ability of the Poisson/gamma to model over-dispersion thus ensured that it was identified as being adequate with considerably greater frequency than the Poisson model.

One unanticipated result occurred at Site 9 (see Tables C.1–C.4). At this site, the Poisson/gamma model was ranked as being the best, yet according to the $\mathcal{D}^3$ measure, this model was inadequate. The Poisson model, ranked fourth, was also deemed to be inadequate. Examination of the data revealed over-dispersion (with an estimated dispersion index equalling 1.75), thus it was not surprising that the Poisson model was inconsistent with this empirical data. However, both the mixture of two Poissons (ranked second) and geometric (ranked third) models were adjudged as being adequate. It seems, therefore, that the Occam's razor[1] (Starfield, Smith and Bleloch, 1990, Jefferys and Berger, 1992) inherently contained within the averaged Bayes factor technique favoured model parsimony over data consistency for those accidents recorded at Site 9.

Evidence indicating inadequacy of the mixture of two Poisson densities model was relatively rare. Indeed, both the $\mathcal{D}^1$ and $\mathcal{D}^3$ measures designated only one site of the 35 as being inadequate, the under-dispersed Site 6. In this instance, model M_3 was ranked third by the averaged Bayes factor, the position this model generally held, and thus this inadequacy is of no great consequence.

On each of the nine occasions that the geometric model rose above the fourth rank, it was never found to be inadequate by any of the three adequacy measures implemented. Nonetheless, the general applicability of this model must be treated with suspicion as it recorded the fourth and worst rank on 26 (74%) occasions and was demonstrated to be inadequate at 13 (37%) and 14 (40%) sites by the $\mathcal{D}^1$ and $\mathcal{D}^3$ adequacy measures, respectively.

[1]Named after a fourteenth century English philosopher William of Occam (or Ockham) who propounded a heuristic in Latin "*Non sunt multiplicanda entia praeter necessitatem*". Translated literally, this means "Things should not be multiplied without good reason", but in the context of model discrimination it means that if two models explain data equally well, the simpler should be preferred.

An alternative explanation for the apparent superiority that the Poisson/gamma and mixture of two Poissons models wield over the Poisson and geometric models, in terms of data compatibility, is due to the lack of sensitivity of the $\mathcal{D}^1$ measure in detecting inadequacy. The lack of sensitivity stemming from the embodiment of pseudo-mean and pseudo-variance values. Calculations of power will enable this conjecture of $\mathcal{D}^1$ measure insensitivity to be quantitatively investigated, and these follow in Section 4.6.2. However, if we just consider the results associated with the $\mathcal{D}^3$ measure (which did not use these pseudo quantities), the Poisson/gamma model was identified as being inadequate at half the number of sites that the Poisson model was found to be inadequate. So, it seems, that the Poisson/gamma model is generally more consistent with these accident data.

Binomial data

We now consider the issue of model adequacy for Site B, hypothetical data derived by generating a sample of 20 independent observations from the $\mathcal{B}(5, \frac{1}{2})$ distribution. To ensure that an atypical generation was not inadvertently selected, its adequacy was checked against the parent distribution using each of the three adequacy measures. At $\alpha = 0.05$, there was no evidence to suspect that this sample was incompatible with the generating distribution.

Results of the adequacy calculations made on the four candidate models for this hypothetical site appear in Table 4.2.

Table 4.2: Observed adequacy measures and associated critical values ($\alpha = 0.05$) of the four candidate models (listed according their averaged Bayes factor rank) on the Site B data using the three discrepancy measures. The symbols c^i and d^i denote $\log \hat{c}_\alpha^i(M_j)$ and $\log d^i(M_j)$ values, respectively, for discrepancy measure i and model M_j.

Model	Rank	d^1	c^1	d^2	c^2	d^3	c^3
M_1	1	1.4*	(2.3, 3.6)	−32.3*	(−46.3, −33.0)	−1.6*	(−1.8)
M_2	2	1.4*	(2.2, 3.3)	−32.7*	(−46.1, −33.5)	−1.6*	(−1.9)
M_3	3	0.5*	(1.4, 3.2)	−32.7*	(−48.9, −33.5)	−1.6*	(−1.9)
M_4	4	−0.1*	(2.0, 3.9)	−45.5	(−58.8, −33.6)	−0.8*	(−1.7)

Note: * denotes *inadequacy* at $\alpha = 0.05$.

The lack of dispersion associated with data contained within Site B lead to the rejection of all the considered models by all the adequacy measures (except, again,

when using the $\mathcal{D}^2$ adequacy measure on the M_4 geometric model). This result is certainly reassuring as we were privileged in knowing that the data actually arose from an under-dispersed binomial distribution.

Analysis of this site, coupled with the results obtained from investigation of Site 6 data, forcefully demonstrates the need for adequacy considerations to be made before discriminated models are employed for analysis. At both Sites 6 and B the Poisson density was assessed as being the most preferred model, yet further exploration revealed that this model was, in actuality, quite inconsistent from the data it was suppose to represent. Bayesian model selection techniques make no explicit statement of the discriminated model's goodness-of-fit with the empirical data.

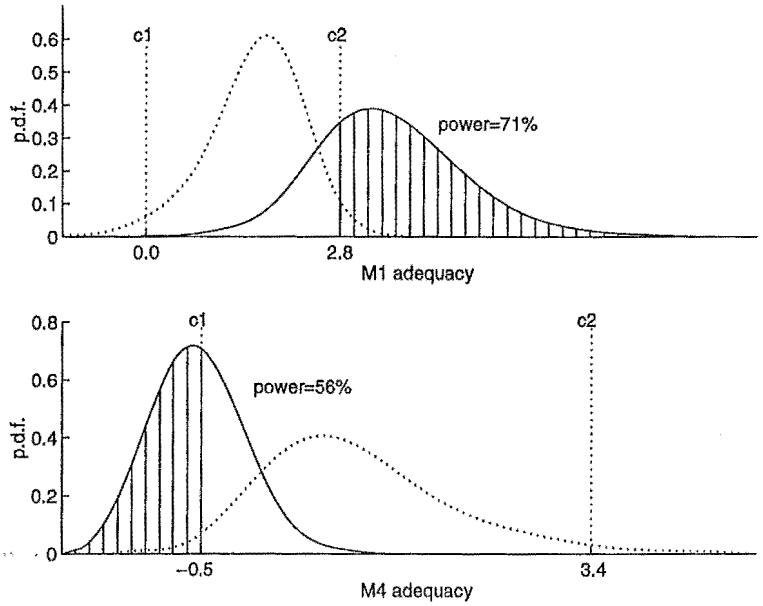
4.6.2 Power of detecting model inadequacy

It was evident from the preceding section that the ability of identifying model inadequacy was not the same for each of the measures considered. Moreover, as the data collection periods were of widely different lengths, it could be surmised that the ability of any given $\mathcal{D}^r$ measure in detecting model inadequacy might vary across sites. This motivated an investigation into detecting the *power* of finding model inadequacy when the model was indeed false.

An assessment of power was achieved by investigating the likelihood that a particular selected model was deemed inadequate when an alternative model, itself generally compatible with the observed data $\boldsymbol{x}$, was taken as the actual underlying distribution. All assessments of power made within this thesis were based upon $\alpha = 0.05$.

Figure 4.3 illustrates a typical simulation scenario computing $\widehat{P}^1(M_1, M_4)$, the power of identifying Poisson model inadequacy when the underlying distribution was geometric (top graph), and $\widehat{P}^1(M_4, M_1)$, the power of identifying geometric model inadequacy when the underlying distribution was Poisson (bottom graph). Both these illustrated power computations were derived using adequacy measure $\mathcal{D}^1$ on Site 1 data. The shaded region gives the region of rejection based on $\alpha = 0.05$ and hence power. For these scenarios, if the data were truly generated by the geometric distribution, we would reject the Poisson assumption 71% of the time; while, if the underlying function was Poisson, then in 56% of instances the geometric adequacy

Figure 4.3: The top graph presents the distribution of $\log \widehat{\mathcal{F}}^{1}(d \mid 1,1)$ and associated critical values for Site 1 data (dotted lines), together with $\log \widehat{\mathcal{F}}^{1}(d \mid 1,4)$ and corresponding power (solid line), while the bottom graph gives the distribution of $\log \widehat{\mathcal{F}}^{1}(d \mid 4,4)$ and associated critical values for Site 1 data (dotted lines), together with $\log \widehat{\mathcal{F}}^{1}(d \mid 4,1)$ and power (solid line).



would be rejected.

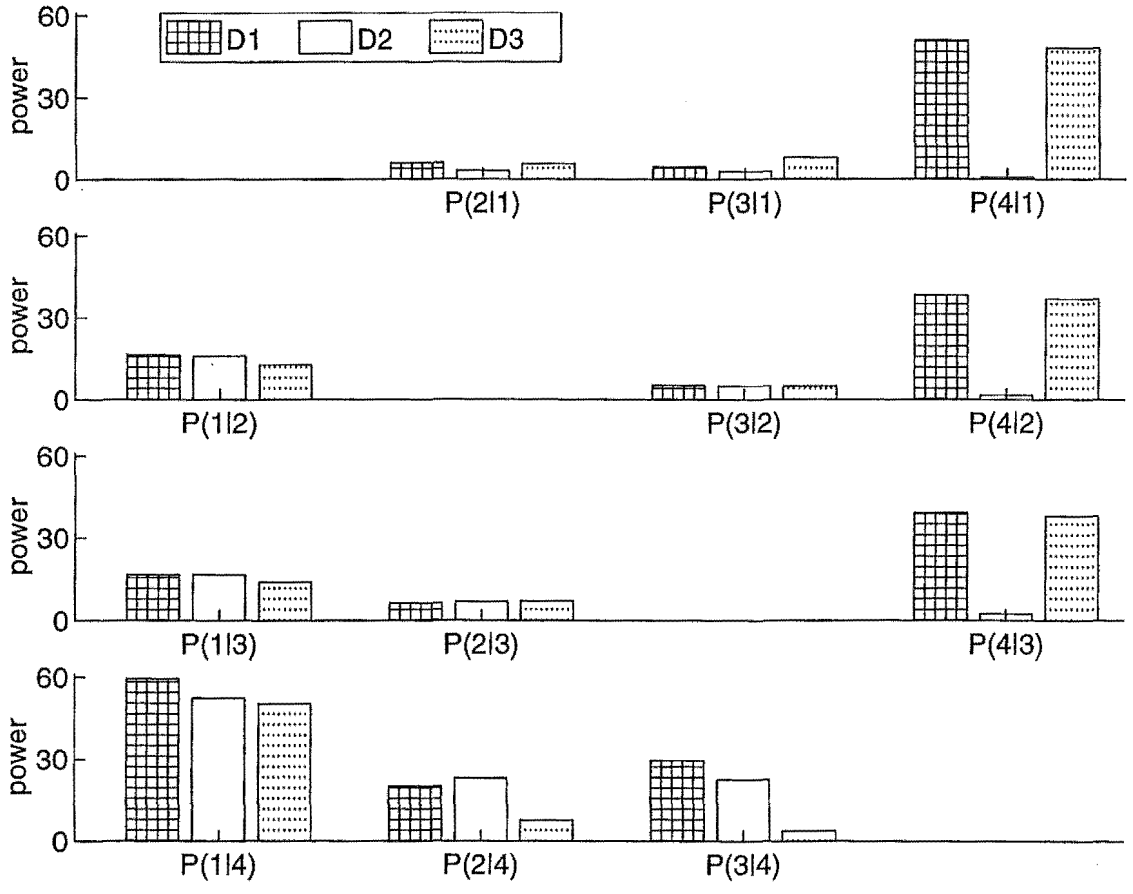
Tables C.5–C.9 included in Appendix C furnish the results of the power calculations defined by (4.9) and (4.10) for the four specified models at each respective accident site. These results are further summarised in Figure 4.4, which presents the power of determining model inadequacy, averaged over the 35 accident sites, for each candidate model. These power estimates were determined by treating, each successively, the three other candidate models as the underlying distribution function.

The adequacy measures

It is apparent from Figure 4.4 that the $\mathcal{D}^1$ measure generally detected model inadequacy with the highest degree of power, despite using pseudo-values to assess the Poisson/gamma and mixture of two Poissons model adequacy. When this $\mathcal{D}^1$ measure was averaged over all the scenarios presented in this figure, the mean power value equalled 24%.

Adequacy measured by $\mathcal{D}^3$ had power that performed with similar consistency, over these scenarios, to that of the $\mathcal{D}^1$ measure except it was, on average, 4% less

Figure 4.4: Power averaged over the 35 accident sites for each candidate model using the three other candidate models, each considered separately, as the underlying distribution. The symbol Dr denotes the power associated with each $\mathcal{D}^r$ measure for $r = 1, 2, 3$ and $\mathrm{P}(i \mid j)$ corresponds to $\overline{P}^r(M_i, M_j)$.



powerful.

Consistency, however, was lacking from the $\mathcal{D}^2$ measures. In one averaged power comparison presented in Figure 4.4, the $\mathcal{D}^2$ measure had power that out performed that associated with either $\mathcal{D}^1$ or $\mathcal{D}^3$ measures and on a further eight occasions, its averaged power was only slightly below the most powerful measure. In contrast, the remaining three comparisons revealed that $\mathcal{D}^2$ identified model inadequacy with exceptionally poor power (frequently 0% or thereabouts). The $\mathcal{D}^1$ and $\mathcal{D}^3$ measures, by comparison, detected model inadequacy for these comparisons with considerable success. This feature resulted in the averaged power across all scenarios for the $\mathcal{D}^2$ equalling 13%, some 11% below that recorded by the $\mathcal{D}^1$ measure.

It is evident that in the three instances the $\mathcal{D}^2$ measure performed poorly, each measured geometric model inadequacy. The reasoning behind this apparent peculiarity is explained in Section 4.6.3.

Model performance

The power of detecting model inadequacy for each of the entertained candidate models, using data known to have arisen from some other underlying alternative distribution, is now examined.

From the bar-graph depiction in Figure 4.4 it is clear that when data were generated from the geometric model and Poisson adequacy was monitored (denoted by P(1 | 4) in this figure), all three measures rejected the applicability of the Poisson model with high power ($\approx 60\%$). Almost equally powerful was the rejection, by the $\mathcal{D}^1$ and $\mathcal{D}^3$ measures, of geometric adequacy when the underlying distribution was Poisson (represented by P(4 | 1) in Figure 4.4). In fact, both the $\mathcal{D}^1$ and $\mathcal{D}^3$ measures detected geometric inadequacy with high degrees of power for data generated from all three alternative candidate models entertained: Poisson; Poisson/gamma; and the mixture of two Poissons (represented by P(4 | 1), P(4 | 2), and P(4 | 3) in Figure 4.4, respectively).

None of the reported measures yielded power of any substance when investigating Poisson/gamma or mixture of two Poisson inadequacy from Poisson, Poisson/gamma and the mixture of two Poissons underlying models. In these scenarios the resultant power was typically around 5%, the α level. Poisson model inadequacy under either the Poisson/gamma (given by P(1 | 2)) or the mixture of two Poissons (given by

P(1 | 3)) was, however, considerably higher with an average of approximately 16% for each of the three measures used.

Binomial data

Power associated with detecting model inadequacy for the Site B data was next considered and associated results appear in Table 4.3. Perusal of this table reveals

Table 4.3: Power(%) for each candidate model, given Site B data, using the three other candidate models and the binomial $\mathcal{B}(n = 5, p = \frac{1}{2})$ model, each considered separately, as the underlying distribution. The symbol $P^r_{j|i}$ denotes $\widehat{P}^r(M_j, M_i)$.

i	$P^1_{1\|i}$	$P^2_{1\|i}$	$P^3_{1\|i}$	$P^1_{2\|i}$	$P^2_{2\|i}$	$P^3_{2\|i}$	$P^1_{3\|i}$	$P^2_{3\|i}$	$P^3_{3\|i}$	$P^1_{4\|i}$	$P^2_{4\|i}$	$P^3_{4\|i}$
1	·	·	·	5	5	7	3	3	6	95	0	89
2	7	7	6	·	·	·	3	3	6	92	0	86
3	11	10	9	10	10	9	·	·	·	91	1	86
4	94	83	85	46	56	7	70	46	5	·	·	·
B	49	49	28	52	48	36	57	51	37	100	0	100

that sizeable power exists, in finding each of the four candidate models as being inadequate, by the three adequacy measures when the data arose from the under-dispersed $\mathcal{B}(5, \frac{1}{2})$ distribution. Exception to generality occurred when $\widehat{P}^2(M_4, M_B)$ was considered, reflecting a deficiency in the $\mathcal{D}^2$ measure in testing for geometric model inadequacy on under-dispersed data. Notice that $\widehat{P}^2(M_4, M_B) = 0\%$, a value in complete contrast to the 100% power achieved using the either of the $\mathcal{D}^1$ or $\mathcal{D}^3$ adequacy measures.

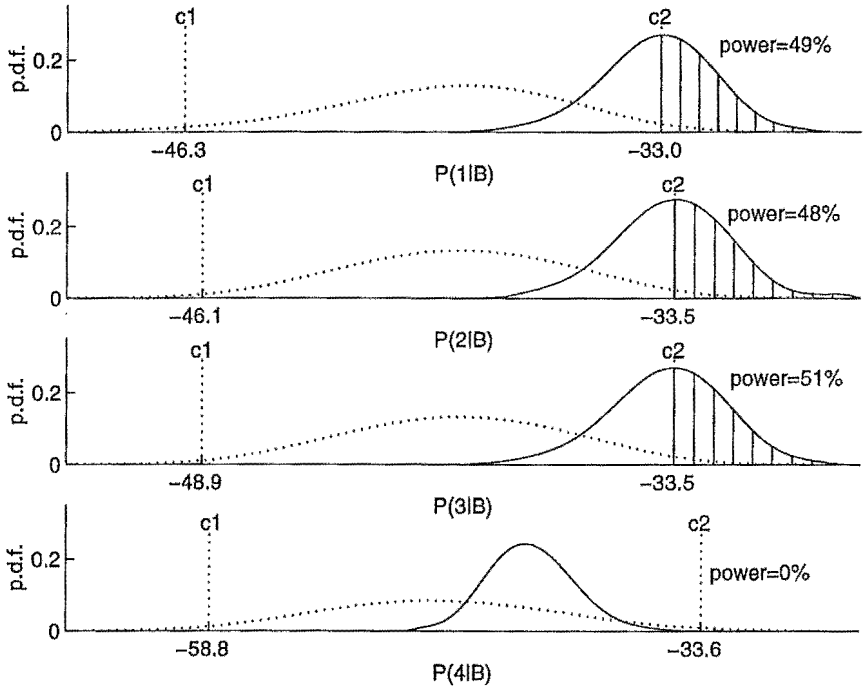
The trends contained in Table 4.3 were entirely consistent with those previously observed using the accident data from the 35 sites and depicted in Figure 4.4.

4.6.3 The $\mathcal{D}^2$ adequacy measure

As portrayed in Figure 4.5, when some alternative underlying distribution M_k generates data, as opposed to the assumed M_j distribution, then the associated distribution of $\log \widehat{\mathcal{F}}^2(d \mid j, k)$ is usually shifted either to the right (as demonstrated in the top three graphs of Figure 4.5) or to the left of the $\log \widehat{\mathcal{F}}^2(d \mid j, j)$ distribution. The magnitude of this shift directly relates to the magnitude of power for

detecting model inadequacy. However, this sideways movement does not appear to have eventuated when geometric adequacy was investigated, i.e. $\log \widehat{\mathcal{F}}^2(d \mid 4, k)$, $k = 1, 2, 3, B$. In particular, when the binomial $\mathcal{B}(5, \frac{1}{2})$ model generated the data, the $\mathcal{D}^2$ measure had 0% power in detecting geometric (M_4) inadequacy (bottom graph of Figure 4.5). This characteristic was unexpected and unsettling because the under-dispersed binomial data were considerably different to that anticipated from a geometric model.

Figure 4.5: The p.d.f.'s of $\log \widehat{\mathcal{F}}^2(d \mid j, j)$ and associated critical values using Site B data for $j = 1, 2, 3, 4$ (dotted lines), together with the p.d.f. of $\log \widehat{\mathcal{F}}^2(d \mid j, B)$ and corresponding power when the data were generated by the $\mathcal{B}(5, \frac{1}{2})$ density (solid lines). The symbol P(i | B) corresponds to the graph presenting $\widehat{P}^2(M_i, M_B)$.

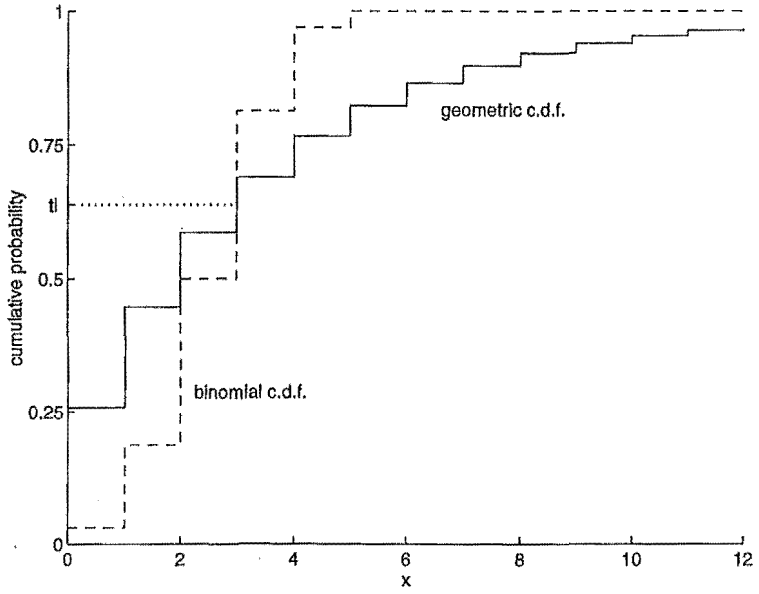


To understand why this characteristic manifests this $\mathcal{D}^2$ measure, we need to recall certain properties of the geometric distribution; namely, it is always anchored with modal value at zero and it has a long monotonically decreasing probability density function (as seen in Figure 4.6). These features combine to give an adequacy distribution $\mathcal{F}^2(d \mid 4, k)$ for $\mathcal{D}^2$ that is so broad that the power to discern between the geometric and other underlying distributions is negligible for the examples presented herein.

We now illustrate this phenomenon by considering the specific example where

geometric adequacy is investigated on data actually originated from $\mathcal{B}(5, \frac{1}{2})$. A similar approach can be applied to describe this behaviour of the $\mathcal{D}^2$ measure when investigating adequacy of the geometric model for the other distributions considered within this thesis.

Figure 4.6: Cumulative predictive distributions of $F_j(y \mid \boldsymbol{x})$, for the geometric model (based on a drawn p^i equalling the M.L.E.) and $\mathcal{B}(5, \frac{1}{2})$ densities conditioned upon the Site B data.



Before power can be estimated, the distribution $\mathcal{F}^2(d \mid 4, 4)$ is required as this gives the regions of rejection. An approximation to $\mathcal{F}^2(d \mid 4, 4)$ is found, according to the proposed simulation scheme, by generating N observations of *replicated* data $\{\boldsymbol{y}_1, \ldots, \boldsymbol{y}_N\}$, each $\boldsymbol{y}_i$ being a vector of length n generated from the posterior predictive distribution $f_4(\boldsymbol{y}_i \mid \boldsymbol{x})$, such that $\boldsymbol{y}_i = (y_{i,1}, \ldots, y_{i,n})$. Recall that this generation was accomplished by generating a p^i variate from the posterior $\pi_4(p \mid \boldsymbol{x})$ and then using this parameter to generate a corresponding $\boldsymbol{y}_i$. All N such observations were derived by repeating this procedure N times.

Power is then determined by computing an approximate $\widehat{\mathcal{F}}^2(d \mid 4, B)$ (where "B" denotes the binomial model) and estimating the area that lies in the rejection region specified from $\widehat{\mathcal{F}}^2(d \mid 4, 4)$. In the bottom graph of Figure 4.5, $\widehat{\mathcal{F}}^2(d \mid 4, B)$ is given by the solid line while $\widehat{\mathcal{F}}^2(d \mid 4, 4)$ is indicated by the dotted line. Notice from this graph that $\widehat{\mathcal{F}}^2(d \mid 4, B)$ is completely contained within $\widehat{\mathcal{F}}^2(d \mid 4, 4)$ and consequently estimated power equals 0%.

We now show that a model (denoted by $\tilde{B}$) which generates replicate data $\boldsymbol{y}_i$ of length n that is geometric from model M_4 (specified by p^i) except for the first data point $y_{i,1}$, which is generated from $\mathcal{B}(5, \frac{1}{2})$, yields an adequacy distribution $\widehat{\mathcal{F}}^2(d \mid 4, \tilde{B})$ generally contained within $\widehat{\mathcal{F}}^2(d \mid 4, 4)$. Because this $\widehat{\mathcal{F}}^2(d \mid 4, \tilde{B})$ has only one binomial value in each n vector of $\boldsymbol{y}_i$ and is generally contained within $\widehat{\mathcal{F}}^2(d \mid 4, 4)$, it follows that $\widehat{\mathcal{F}}^2(d \mid 4, B)$ composed of entirely binomial data must also be contained within $\widehat{\mathcal{F}}^2(d \mid 4, 4)$.

We take, for convenience, $y_{i,1}$ as being the binomial or geometric generated data corresponding to $M_{\tilde{B}}$ and M_4, respectively, (although any term of the n vector could have been chosen).

Suppose that all replicated data are acquired using the inverse generating method[2] (Pidd, 1986) derived from some common randomly generated "u" vector, $u = (u_{i,1}, \ldots, u_{i,n})$, then the following relationships hold. If t_i denotes the value where the c.d.f.'s for both the geometric (specified by p^i) and binomial predictive densities intersect (see Figure 4.6) then, from the adoption of the inverse generating method, $u_{i,1} > t_i$ implies the generated geometric data point is greater than or equal to the generated binomial data point. Because of the monotonically decreasing probability density function associated with the geometric model, this implies, in general, that $D_i^2(M_4, M_4) \leq D_i^2(M_4, M_{\tilde{B}})$ and thus the right hand tail of $\widehat{\mathcal{F}}^2(d \mid 4, \tilde{B})$ is shifted to the left of $\widehat{\mathcal{F}}^2(d \mid 4, 4)$. Similarly, when $u_{i,1} \leq t_i$, then the generated geometric data point is smaller than or equal to the generated binomial data point. This implies, in general, that $D_i^2(M_4, M_4) \geq D_i^2(M_4, M_{\tilde{B}})$ and so the left hand tail of $\widehat{\mathcal{F}}^2(d \mid 4, \tilde{B})$ is shifted to the right of $\widehat{\mathcal{F}}^2(d \mid 4, 4)$.

These features combine to give a distribution $\widehat{\mathcal{F}}^2(d \mid 4, \tilde{B})$ generally contained within $\widehat{\mathcal{F}}^2(d \mid 4, 4)$. Because $\tilde{B}$ has only one binomial data point in each $\boldsymbol{y}_i$ and has corresponding adequacy distribution contained within $\widehat{\mathcal{F}}^2(d \mid 4, 4)$, it follows that replicate data generated entirely from the binomial distribution would also yield an adequacy distribution contained within $\widehat{\mathcal{F}}^2(d \mid 4, 4)$.

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[2]Briefly this technique can be described as follows. Suppose $\mathrm{F}(x)$, a known c.d.f., is randomly assigned a value u, a random variable uniformly distributed on the $[0, 1]$ interval, then any value of u may be transformed into a value x by inverting the c.d.f. and solving for x. Algebraically, if

$$u = \mathrm{F}(x) = \int_0^x f(t)\, dt \quad \text{then} \quad x = \mathrm{G}(u),$$

where $\mathrm{G}(u)$ is the inverse cumulative function.

Chapter 5

Ranking and selection

5.1 Specification of an appropriate model

It was evident, from Table 4.1, that of the four candidate models investigated over the 35 intersection accident sites, the mixture of two Poisson densities was generally the most adequate at $\alpha = 0.05$. It was also apparent that this model was demonstrated as having slightly fewer identifications of model inadequacy to that of the Poisson/gamma model. Comparative to the mixture of two Poisson densities and Poisson/gamma models, in terms of model adequacy, the Poisson model performed considerably worse and the geometric worse still.

Model adequacy does not and should not imply model selection (Upadhyahy and Smith, 1993). Appealing to Occam's razor, it is disadvantageous and inefficient to select overly cumbersomes models containing structural or variable redundancies when more parsimonious models exist that are equally compatible with the data. Adequacy calculations make no consideration of model parsimony. This notion was borne out with the most adequate mixture of two Poisson densities model receiving little support from the averaged Bayes factor model discrimination technique.

Although the most adequate model, the mixture of two Poisson densities lack of parsimony, relative to the three alternative candidate models investigated, suggested that this model could be improved upon.

In contrast, simplicity is a strength of the geometric model. In those situations with considerably dispersed data, this model ably and adequately represented the empirical data, unlike the Poisson model. In most situations, however, the geometric model received little model discrimination favour from the averaged Bayes factor and, as previously observed from Table 4.1, was frequently inadequate.

The averaged Bayes factor favoured the Poisson model more frequently than the Poisson/gamma model, although, at a number of sites the Poisson model did worse, often considerably. As observed in Section 3.4, this phenomenon resulted in the averaged posterior probability over all 35 sites being virtually indistinguishable for both Poisson and Poisson/gamma models with $\overline{P}(M_1 \mid \boldsymbol{x}) = 0.313$ and $\overline{P}(M_2 \mid \boldsymbol{x}) = 0.309$.

The parsimonious strength possessed by the Poisson model, in having only one model parameter, was also its weakness at times, as the Poisson model had difficulty in accommodating over-dispersed data. The consequence of this deficiency, as portrayed in Table 4.1, was that at 23% of the sites (using the $\mathcal{D}^1$ measure) the Poisson model could not adequately represent the empirical data. By comparison, the slightly more complicated but flexible Poisson/gamma model, which recorded inadequacy at only 6% of the sites, demonstrated that it more appropriately handled those over-dispersed scenarios.

On the basis of these results, it appeared that the Poisson/gamma model was more suitable in representing traffic accidents than the Poisson model; at least for the data presented in Table A.1. We thus conduct hazardous site ranking and selection with the embodiment of the Poisson/gamma statistical model.

5.2 Hierarchical Bayesian development

The objective is to select the site, or sites, that are most hazardous. As the determination of such hazardous sites requires the simultaneous investigation and comparison of accident sites, new notation must be defined to accommodate this situation, which follows.

Let $x_{i1}, x_{i2}, \ldots, x_{in_i}$ represent the observed accident counts measured for a period n_i at the i^{th} accident site for $i = 1, 2, \ldots, K$. Furthermore, let $\boldsymbol{x} = (x_1, x_2, \ldots, x_K)$, where $x_i = \sum_{j=1}^{n_i} x_{ij}$, denote the vector of summed observations from the K sites. Suppose also that the K accident sites are independent.

Adopting the model recommendations drawn in Section 5.1, we presume that the observed data x_{ij}, at each site, can be described by the Poisson distribution and that each accident site has underlying accident rate λ_i, with $\lambda_i > 0$. Noting the distribution of a sum of independent Poisson distributed random variables is itself a Poisson random variable with parameter equal to the sum of the individual parameters, then the distribution describing the summed accidents, x_i, for each site conditional on λ_i is given by

$$f(x_i \mid \lambda_i) = \frac{(n_i\lambda_i)^{x_i} e^{-n_i\lambda_i}}{x_i!} \tag{5.1}$$

for $i = 1, 2, \ldots, K$ and $\lambda_i > 0$.

The Bayesian method specifies that these λ_i's, $\boldsymbol{\lambda} = (\lambda_1, \lambda_2, \ldots, \lambda_K)$, are a realisation from some common prior distribution $\pi(\boldsymbol{\lambda})$, and the hierarchical Bayesian approach seeks to place a *second stage* subjective prior on the parameters of $\pi(\boldsymbol{\lambda})$.

From the investigations of Chapters 3 and 4, and summary contained in Section 5.1, it is evident that prior information is suitably modelled by assuming that the λ_i's are a random sample from some conjugate gamma distribution. To facilitate the elicitation of prior information, the gamma distribution is reparametrised from that adopted in Section 2.1 with

$$\pi(\lambda_i \mid \beta, \eta) = g(\lambda_i \mid \frac{\beta}{\eta}, \frac{1}{\eta}), \tag{5.2}$$

for $\beta > 0$ and $\eta > 0$, where

$$g(y \mid a, b) = \frac{b^a}{\Gamma(a)} y^{a-1} e^{-by}$$

is the notation for the gamma distribution for $a > 0$ and $b > 0$. The prior distribution on $\boldsymbol{\lambda}$ can then be written as

$$\pi(\boldsymbol{\lambda}) = \int_\eta \int_\beta \pi(\boldsymbol{\lambda} \mid \beta, \eta)\, h(\beta, \eta)\, d\beta\, d\eta, \tag{5.3}$$

where

$$\pi(\boldsymbol{\lambda} \mid \beta, \eta) = \prod_{i=1}^{K} \pi(\lambda_i \mid \beta, \eta),$$

which assures the underlying important quantities $\lambda_1, \ldots, \lambda_K$ are exchangeable. We remark that the assumption of exchangeability is important in modelling prior opinion about these quantities and that the representation above is but one of many forms which assure exchangeability.

The particular form of $\pi(\lambda_i \mid \beta, \eta)$ given by (5.2) facilitates the elicitation of prior information about β and η due to the mean and variance relationships

$$\mathrm{E}[\lambda_i \mid \beta, \eta] = \beta \quad \text{and} \quad \sigma^2 = Var(\lambda_i \mid \beta, \eta) = \eta\beta. \tag{5.4}$$

The hierarchical structure then consists of placing prior distribution $h(\beta, \eta)$, called the 'hyperprior density', on the unknown hyperparameters. It will be convenient to determine $h(\beta, \eta)$ by adopting the conditional relationship between the hyperparameters β and η of the form

$$h(\beta, \eta) = h_2(\eta \mid \beta)\, h_1(\beta). \tag{5.5}$$

Hyperprior density $h_1(\beta)$ will be taken as a member of the gamma family, $g(\beta \mid a, b)$, and the hyperprior density over η is defined by

$$h_2(\eta \mid \beta) = \begin{cases} \dfrac{m\beta}{(m+1)\, c} & 0 < \eta \leq c/\beta \\ \\ \dfrac{m\beta\, c^m}{(m+1)(\eta\beta)^{m+1}} & c/\beta < \eta. \end{cases} \tag{5.6}$$

The values of the parameters for $h_1(\beta)$ and $h_2(\eta \mid \beta)$ depend upon what prior information is available and are discussed in more detail in Section 5.4.

Using the notation and assumptions of above, the distribution of x_i given the hyperparameters β and η can be expressed by

$$\begin{aligned} f(x_i \mid \beta, \eta) &= \int_0^\infty f(x_i \mid \lambda_i)\, \pi(\lambda_i \mid \beta, \eta)\, d\lambda_i \\ \\ &= \frac{(1/\eta)^{\beta/\eta} n_i^{x_i}}{\Gamma(\beta/\eta)\, x_i!} \int_0^\infty \lambda_i^{(x_i+\beta/\eta)-1} e^{-\lambda_i(n_i+1/\eta)}\, d\lambda_i \end{aligned}$$

and exploiting the gamma distribution providing $x_i + \beta/\eta > 0$ and $n_i + 1/\eta > 0$, which is assured because $\beta > 0$ and $\eta > 0$, then

$$\begin{aligned} f(x_i \mid \beta, \eta) &= \frac{(1/\eta)^{\beta/\eta} n_i^{x_i}}{\Gamma(\beta/\eta)\, x_i!} \frac{\Gamma(x_i + \beta/\eta)}{(n_i + 1/\eta)^{x_i+\beta/\eta}} \\ \\ &= nb\left(x_i \mid \frac{1}{1+\eta n_i}, \frac{\beta}{\eta}\right) \end{aligned} \tag{5.7}$$

in which

$$nb(y \mid a, b) = \begin{pmatrix} y+b-1 \\ y \end{pmatrix} a^b(1-a)^y$$

denotes the negative binomial distribution for $a > 0$ and $b > 0$. As the data are assumed to be conditionally independent

$$f(\boldsymbol{x} \mid \beta, \eta) = \prod_{i=1}^{K} f(x_i \mid \beta, \eta) \tag{5.8}$$

so the full marginal distribution of the data can be expressed by

$$f(\boldsymbol{x}) = \int_0^\infty \int_0^\infty f(\boldsymbol{x} \mid \beta, \eta)\, h_2(\eta \mid \beta)\, h_1(\beta)\, d\beta\, d\eta. \tag{5.9}$$

Using Bayes theorem and (5.7), it is easy to see that

$$\begin{aligned} \pi(\lambda_i \mid x_i, \beta, \eta) &= \frac{f(x_i \mid \lambda_i)\, \pi(\lambda_i \mid \beta, \eta)}{f(x_i \mid \beta, \eta)} \\ &= g(\lambda_i \mid x_i + \frac{\beta}{\eta}, n_i + \frac{1}{\eta}) \end{aligned} \tag{5.10}$$

and it follows that the distribution of $\boldsymbol{\lambda}$ conditional on $\boldsymbol{x}$, β and η is given by

$$\pi(\boldsymbol{\lambda} \mid \boldsymbol{x}, \beta, \eta) = \prod_{i=1}^{K} g(\lambda_i \mid x_i + \frac{\beta}{\eta}, n_i + \frac{1}{\eta}). \tag{5.11}$$

The posterior distribution of $\boldsymbol{\lambda}$ given the data $\boldsymbol{x}$ can then be expressed as

$$\pi(\boldsymbol{\lambda} \mid \boldsymbol{x}) = \int_0^\infty \int_0^\infty \pi(\boldsymbol{\lambda} \mid \boldsymbol{x}, \beta, \eta)\, \frac{f(\boldsymbol{x} \mid \beta, \eta)}{f(\boldsymbol{x})}\, h_2(\eta \mid \beta)\, h_1(\beta)\, d\beta\, d\eta. \tag{5.12}$$

It will be the case that the precise form of this posterior will not be required since decisions about which accident site, or subset of accident sites, that should be selected are based on easily computed expectations taken with respect to this posterior distribution.

5.3 Selection criteria

In this thesis we propose three new criteria for determining which accident site is worst, using: the posterior probability; the predictive probability; and the posterior mean. Within each criterion there exist two intuitively appealing approaches that select hazardous sites from the collection under investigation, namely:

1. Stipulate a number of sites, r, to be deemed hazardous, for $r < K$. Upon application of the appropriate selection criterion, find the subgroup that contains the r most hazardous sites.

2. After specifying levels which are considered dangerous for the practical situation and appropriate selection criteria, select those sites that exceed the designated threshold values.

Strategy (1) regulates selection numbers but ignores accident hazard potential for those sites not selected. This approach would appeal to those who diagnose problems, identify potential countermeasures, and select appropriate remedial treatments, but have constrained resources thereby restricting their investigation into a maximum of r sites over a given time. Stratagem (2) ensures selection of sites deemed hazardous at some critical level, but leaves variable the number of sites that may be selected. Should policy decree, say, that sites having at least 50% chance of exceeding 5 accidents per year must require investigation, then strategy (2) is clearly the more appropriate selection approach.

As suggested, implementation of a specific selection criterion depends upon the requirements of the practitioner for the given situation; each criterion is now described below.

5.3.1 Posterior probability of selecting the worst site

The first criterion we propose is the posterior probability that the underlying accident rate of one site is larger than the underlying accident rates of the remaining sites by a positive multiple 'v'. Mathematically, let

$$p_i(v) = P(\lambda_i > \lambda_j v \text{ for all } i \neq j \mid \boldsymbol{x}) \tag{5.13}$$

where $v \in [0, \infty]$. When $v = 1$, $p_i(v)$ is simply the posterior probability that λ_i is the largest; hence $\sum_{i=1}^{K} p_i(1) = 1$. For $v > 1$ the posterior probability represents an expression of just how much worse one accident site is compared to all the others. Note that this calculation is required for each of the K sites within the group.

Selection is made by either: (1) selecting the r largest $p_i(v)$ values, $i = 1, \ldots, K$, for a particular v; or (2) obtained by taking the smallest subgroup of sites with summed $p_i(v)$ values that exceeds some threshold value, say P^*, for $i = 1, \ldots, K$

and v. Should no one accident site, or subgroup of sites, differ sufficiently from the remaining accident sites for $v > 1$, then the practitioner may reconsider their parameter specifications either by decreasing the v margin or by lowering the probability requirement. Note, for $v \neq 1$ it is no longer the case that $\sum_{i=1}^{K} p_i(v)$ equals unity.

Invoking (5.1) – (5.8), the formula which allows numerical calculation of the $p_i(v)$'s is seen to be

$$\begin{aligned} p_i(v) &= \int_{A_i(v)} \pi(\boldsymbol{\lambda} \mid \boldsymbol{x})\, d\boldsymbol{\lambda} \\ &= \int_0^\infty \int_0^\infty \left[\int_0^\infty \prod_{j=1, i\neq j}^{K} \mathcal{G}(\frac{\lambda_i}{v} \mid s_j, r_j)\, g(\lambda_i \mid s_i, r_i)\, d\lambda_i \right] \frac{f(\boldsymbol{x} \mid \beta, \eta)}{f(\boldsymbol{x})}\, h(\beta, \eta)\, d\eta\, d\beta \end{aligned} \tag{5.14}$$

where $A_i(v) = \{\boldsymbol{\lambda} : \lambda_i > \lambda_j v \text{ for all } j \neq i\}$, $s_i = x_i + (\beta/\eta)$, $r_i = n_i + (1/\eta)$, and '$\mathcal{G}$' represents the cumulative density function (c.d.f.) of the gamma distribution. Thus to compute $p_i(v)$, for each site, we simply have to evaluate a 3–dimensional integral, provided an incomplete gamma function is available.

5.3.2 Predictive probability of future accident numbers

Suppose that the random variable Y_i denotes the number of accidents in the next period at site i. The second selection criterion we propose is based on the Bayesian predictive probability of Y_i and is defined as

$$pd_i(n_0) = P(Y_i \geq n_0 \mid \boldsymbol{x}) \tag{5.15}$$

for pre-specified n_0, such that $n_0 \in \boldsymbol{Z}^+$. The variable n_0 represents, to the practitioner, an important future accident number, and the probability computation indicates the site's likelihood of having at least n_0 accidents in the next time period.

Selection is made by either: (1) selecting the r largest $pd_i(n_0)$ values, $i = 1, \ldots, K$, for a particular n_0; or (2) by taking those sites, for $i = 1, \ldots, K$, with $pd_i(n_0)$ greater than some threshold value, say P_0, at a specified n_0. For a particular $n_0 > 0$, no accident site may realise a predictive probability greater than some threshold value P_0. In this instance the experimenter may reconsider the n_0 level or reduce the probability requirement P_0.

Using (5.1) – (5.8), and noting that

$$P(Y_i \geq n_0 \mid \boldsymbol{x}) = \int P(Y_i \geq n_0 \mid \boldsymbol{\lambda}, \boldsymbol{x})\, \pi(\boldsymbol{\lambda} \mid \boldsymbol{x})\, d\boldsymbol{\lambda}$$

then the formula required to calculate these predictive probabilities, for $n_0 \geq 1$, is given by

$$pd_i(n_0) = \int_0^\infty \int_0^\infty \left[1 - \sum_{y=0}^{n_0-1} nb(y \mid s_i, r_i)\right] \frac{f(\boldsymbol{x} \mid \beta, \eta)}{f(\boldsymbol{x})}\, h(\beta, \eta)\, d\beta\, d\eta \qquad (5.16)$$

where $s_i = (1 + \eta n_i)/(1 + \eta + \eta n_i)$, and $r_i = x_i + (\beta/\eta)$. Here the computation requires evaluation of only a 2–dimensional integral. For $n_0 = 0$, the predictive probability the next period has at least 0 accidents, $pd_i(0) = 1$.

5.3.3 Expected number of future accidents

The third and final criterion for comparing accident sites uses the average accident rate given the observed data, commonly referred to as the posterior mean, and is derived as follows:

$$\mathrm{E}[\lambda_i \mid \boldsymbol{x}] = \int_0^\infty \lambda_i\, \pi(\lambda_i \mid \boldsymbol{x})\, d\lambda_i.$$

The posterior mean is a point estimate of the underlying accident rate. This mean also usefully provides the expected accident numbers over the long term. For instance, suppose $\mathrm{E}[\lambda_i \mid \boldsymbol{x}] = 3.1$, then in 10 years 31 accidents are expected at site i.

Selection is made by either: (1) selecting the r largest $\mathrm{E}[\lambda_i \mid \boldsymbol{x}]$ values, $i = 1, \ldots, K$; or (2) through determining which sites have $\mathrm{E}[\lambda_i \mid \boldsymbol{x}]$ values that exceed some threshold value, say h, for $i = 1, \ldots, K$.

Again employing (5.1) – (5.8), we can write

$$\mathrm{E}[\lambda_i \mid \boldsymbol{x}] = \int_0^\infty \int_0^\infty \left[\frac{\beta}{1 + \eta n_i} + \frac{\eta n_i}{1 + \eta n_i}\left(\frac{x_i}{n_i}\right)\right] \frac{f(\boldsymbol{x} \mid \beta, \eta)}{f(\boldsymbol{x})}\, h(\beta, \eta)\, d\eta\, d\beta \qquad (5.17)$$

which is an easily calculated 2–dimensional numerical integral.

5.3.4 Appropriate use of selection criteria

Proposed in this thesis are three selection criteria, namely $p_i(v)$, $pd_i(n_0)$ and $\mathrm{E}[\lambda_i \mid \boldsymbol{x}]$; their appropriate use is governed by the practical situation and requirements of the practitioner. Should the practitioner's objective be to reduce accident numbers in

the next immediate time period then selection based upon the predictive probability $pd_i(n_0)$ criterion is most appropriate. Calculations of $pd_i(n_0)$ specifically concentrate on the probability of future accident numbers in the next period, hence are clearly applicable when short term goals are to be achieved. If, however, selection decisions are to be made for the long term then either the $p_i(v)$ or $\mathrm{E}[\lambda_i \mid \boldsymbol{x}]$ criteria are suitable. While calculations involving $\mathrm{E}[\lambda_i \mid \boldsymbol{x}]$ are computationally easier than $p_i(v)$, the posterior probability allows more flexibility with the specification of a distance measure 'v' and provides more intuitive probabilistic answers.

The criteria above contrast markedly to the situation where a conventional test of hypothesis is undertaken in an attempt to determine whether fluctuations between accident sites are due to chance or some underlying difference. Hypothesis tests of this nature often yield statistically inconclusive results. Hence, the practitioner has no statement as to which site, or subset of sites, is worst nor is there any assertion about the *magnitude of difference between sites*. Our criteria suggested above address these deficiencies and give the practitioner intuitively appealing procedures upon which appropriate decisions specific to their practical situation can be made. The analyses contained within Section 5.5 on the accident data presented in Table A.1 will indicate how our criteria compare and are computed.

5.4 Hyperprior distributions and elicitation

The situation arises where practitioners consider that they have sufficient information to specify precise values for β and η in $\pi(\boldsymbol{\lambda} \mid \beta, \eta)$ defined by (5.11); for example, see Hauer (1986). Specific forms of the prior distribution for the unknown parameters $\boldsymbol{\lambda}$ are thus derived. Alternatively, some assume that each λ_i is generated by a unique 'prior' distribution with unknown parameters β_i and η_i, an approach generally referred to as the naive empirical Bayesian model. Past history is frequently used to estimate these unknown parameters. Both of the above approaches are generally quite unrealistic for reasons expounded in Deely and Lindley (1981) and Deely and Gupta (1988). A more realistic approach utilises the notion of exchangeability amongst the λ_i's, a technique detailed in Berger (1985) and Deely and Gupta (1988). Our approach is to exploit this notion of exchangeability and use elicitation to construct informative hyperprior distributions. It may be that such

prior information is not available for this elicitation procedure to be effective so that a noninformative hyperprior distribution is more appropriate. We discuss both of these situations below.

5.4.1 Informative hyperpriors

There are essentially two phases in constructing informative hyperprior densities that model the type of prior information we envisage is available from the practitioner. The first, part 1, requires elicitation from the practitioner of their prior knowledge about the accident sites as a *group*. The second, part 2, requires the adoption of hyperprior distributions that adequately describe the elicited information.

For part 1, we will use the response to the following questions:

1. *Where do you expect the average of the λ_i's to be?*
   That is, can you specify an interval, (s_1, t_1), where you believe that the *average* underlying accident rate for the group of sites will lie within?

2. *How variable do you consider the λ_i's to be?*
   That is, can you specify an interval, (s_2, t_2), where you believe *all* the underlying accident rates for the group of sites will lie within?

It should be emphasised that these questions address quite different aspects of the uncertainty about β and η. The first question elicits the practitioner's belief as to the location of the *mean* underlying accident rate amongst the group so that a distribution on β can be ascertained. The second question gleans practitioner belief about the bounds for the group of underlying accident rates and thus provides information about the prior variance $\eta\beta$. Clearly this implies $s_2 \leq s_1$ and $t_2 \geq t_1$.

For part 2 we need to determine the parameters of the hyperprior density, as given in (5.6). Answers elicited from question 1 enable the determination of $h_1(\beta)$, here taken as a member of the gamma distribution with mean equated to the mid point of the interval (s_1, t_1) and variance $[(t_1 - s_1)/4]^2$. This choice of $h_1(\beta)$ provides a rich form capable of describing a wide variety of circumstances.

Answers to question 2 permits specification of the parameters for $h_2(\eta \mid \beta)$. Using the solicited information an appropriate distribution on σ^2 (see (5.4)), the conditional variance of λ_i given β and η, can be initially obtained. Since the elicited

information expresses a bound, c, on σ^2, we take this to imply a flat distribution on the interval $(0, c)$. However the possibility that the variance could exceed this value is permitted and is modelled with a distribution that decays exponentially to 0. This distribution, used previously in Deely and Zimmer (1988), is called the 'shoe' distribution and is given by

$$f(\sigma^2) = \begin{cases} \dfrac{m}{(m+1)\,c} & 0 < \sigma^2 \leq c \\ \\ \dfrac{mc^m}{(m+1)(\sigma^2)^{m+1}} & c < \sigma^2 \end{cases}$$

where $c = [(t_2 - s_2)/4]^2$ and m is chosen so that $P(0 < \sigma^2 \leq c)$ describes the confidence of the practitioner. Observe that $P(0 < \sigma^2 \leq c) = m/(m+1)$, so an estimate of m is easily attained. Transforming this distribution on σ^2, using $\eta = \sigma^2/\beta$, the distribution of $h_2(\eta \mid \beta)$ as given in (5.6) is readily obtained.

We notice that the responses elicited from questions 1 and 2 could be modelled in other ways besides the one described above. In this thesis, for comparison purposes, we consider one other interpretation; namely, where the responses to questions 1 and 2 provide merely *bounds* on the hyperparameters. This approach we label Case II, while the first discussed hyperprior specification we term Case I.

5.4.2 Noninformative hyperpriors

When the practitioner has insufficient information to adequately respond to questions 1 and 2 it is appropriate to use noninformative hyperpriors for $h(\beta, \eta)$. The manner this is done depends upon ensuring that the posterior distribution is a proper pdf. The simplest form for the noninformative case, that is $h(\beta, \eta) \equiv 1$, does not yield a proper posterior. A proper posterior distribution results, however, when a quasi-noninformative uniform distribution is adopted. As the name suggests, the quasi-noninformative uniform distribution simply implies that each hyperparameter is distributed uniformly over a very large support. The upper bounds of these uniform densities are large but finite, ensuring that a proper posterior distribution results. This hyperprior distribution has support so large that simulation procedures can not discriminate between it and a uniform distribution on a larger bounded support.

It could be suggested that a noninformative hyperprior should be deduced using a method such as Jeffreys (Section 2.2). Here, this approach leads to complicated expressions of little practical use.

Another alternative noninformative hyperprior assumes that $\eta \sim IG(a, b)$, where $IG(a, b)$ is the inverse gamma distribution with density $b^a e^{-b/\eta}/\eta^{a+1}\Gamma(a)$ and parameters $a > 0$ and $b > 0$, and β is assigned some constant value (see Gelfand and Smith (1990) for example). Noninformity results by taking a and b to be very small, perhaps 0. In the noninformative setting, assignment of hyperparameter β is frequently inconvenient or impossible thereby reducing the flexibility and general applicability of this hyperprior.

It might also be suggested that reparameterising with $\mu = \beta$ and $\sigma^2 = \eta\beta$, then adopting the location and scale invariance technique described in Berger (1985) so that $h(\mu, \sigma^2) = 1/\sigma^2$, could be used. This approach, in this instance, does not yield a proper posterior for all $\boldsymbol{x}$.

It will be shown in Section 5.5 that our quasi-noninformative uniform distribution is a reasonable choice for the noninformative case.

5.5 Numerical example

In Section 5.5.2 we consider analyses, designated by Case I, where responses gleaned from questions 1 and 2 are interpreted so that unique members of the gamma and family (5.6) are determined respectively for $h_1(\beta)$ and $h_2(\eta \mid \beta)$. For comparison purposes three different sets of hypothetical answers to questions 1 and 2 are applied, mimicking varying strengths of prior belief potentially held by the practitioner, in addition to the quasi-noninformative hyperprior distribution. For each of these scenarios the three selection criteria advocated in Section 5.3 are then computed.

In Section 5.5.3 we interpret the second hypothetical set of answers to questions 1 and 2 in such a way as to merely put bounds on the hyperparameters; these calculations we denote by Case II. When the broadest interpretation of this information is considered the results obtained from each of the three selection criteria are so diverse that they are of little practical use. However, as will be seen in the latter of Section 5.5.3, the inclusion of additional information compensates for this and yields selection criteria results that are useful.

5.5.1 Computation

Direct Monte Carlo simulation, as employed by Berger and Deely (1988), that is based on the hierarchical representation for the posterior distribution was employed in numerical computations. This method entails generation of a sequence $({}_\iota\beta,\ {}_\iota\eta,\ {}_\iota\lambda_i),\ \iota = 1, \ldots, N$, of independent random vectors; here $({}_\iota\beta,\ {}_\iota\eta)$ are generated according to $h(\beta, \eta \mid \boldsymbol{x})$ and ${}_\iota\lambda_i$ according to $\pi(\lambda_i \mid {}_\iota\beta,\ {}_\iota\eta, \boldsymbol{x})$, so that

$$\mathrm{I} = \int\int\int \Psi(\lambda_i, \beta, \eta, \boldsymbol{x})\, \pi(\lambda_i \mid \beta, \eta, \boldsymbol{x})\, h(\beta, \eta \mid \boldsymbol{x})\, d\lambda_i\, d\eta\, d\beta$$

can be approximated by

$$\hat{\mathrm{I}} = \frac{1}{N} \sum_{\iota=1}^{N} \Psi(\lambda_i, \beta, \eta, \boldsymbol{x}).$$

Generation of ${}_\iota\lambda$ is easily accomplished as $\pi(\lambda_i \mid {}_\iota\beta,\ {}_\iota\eta, \boldsymbol{x})$ has a gamma density. The complicated configuration of distribution $h(\beta, \eta \mid \boldsymbol{x})$ means that generation of ${}_\iota\beta$ and ${}_\iota\eta$ depended on the specific form of $h(\beta, \eta)$.

Acquisition of the necessary ${}_\iota\beta$ and ${}_\iota\eta$ samples arose on implementation of the following stratagem: when $h(\beta, \eta)$ was a proper density with an identifiable upper bound then application of the sampling–resampling scheme, delineated in Smith and Gelfand (1992), provided the sample; the weighted bootstrap technique, again delineated by Smith and Gelfand (1992), was applied with proper $h(\beta, \eta)$ densities but in the absence of an identifiable upper bound; and when $h(\beta, \eta)$ was improper, having infinite mass, or when the quasi-noninformative uniform distribution was employed then the Metropolis algorithm, as detailed in Müller (1991) and Smith and Roberts (1993), was used to acquire samples from $h(\beta, \eta \mid \boldsymbol{x})$.

In using the Metropolis algorithm it has been recognised that good initial estimates improve convergence; Müller (1991) recommends the posterior mode to estimate the unknown parameters and the negative Hessian evaluated at this mode to estimate the covariance matrix. Here, recalling (5.3) with $\mathrm{E}[\lambda_i \mid \beta, \eta] = \beta$ and $\sigma^2 = Var(\lambda_i \mid \beta, \eta) = \eta\beta$, a convenient (and intuitive) estimation technique equates the observed moments of the data to the unknown parameters, so that

$$\tilde{\beta} = \frac{1}{K} \sum_{i=1}^{K} \frac{x_i}{n_i} = \bar{\lambda}$$

and

$$\tilde{\eta} = \frac{\hat{\sigma}^2}{\tilde{\beta}} = \frac{1}{\tilde{\beta}\, K} \sum_{i=1}^{K} \left(\frac{x_i}{n_i} - \bar{\lambda} \right)^2.$$

The covariance matrix Σ has several components, all of which require estimation, namely; the variance of β, σ_β^2, the variance of η ,σ_η^2, and ρ the covariance between β and η, so

$$\tilde{\Sigma} = \begin{bmatrix} \hat{\sigma}_\beta^2 & \hat{\rho}\hat{\sigma}_\beta\hat{\sigma}_\eta \\ \hat{\rho}\hat{\sigma}_\beta\hat{\sigma}_\eta & \hat{\sigma}_\eta^2 \end{bmatrix}.$$

Convenient estimates can be obtained by randomly partitioning sites into J subgroups each of size K_j, $j = 1, \ldots, J$, then estimating $\tilde{\beta}_j$ and $\tilde{\eta}_j$ by

$$\tilde{\beta}_j = \frac{1}{K_j} \sum_{i=1}^{K_j} \frac{{}_jx_i}{{}_jn_i} = \bar{\lambda}_j$$

and

$$\tilde{\eta}_j = \frac{\hat{\sigma}_j^2}{\tilde{\beta}_j} = \frac{1}{\tilde{\beta}_j\, K_j} \sum_{i=1}^{K_j} \left(\frac{{}_jx_i}{{}_jn_i} - \bar{\lambda}_j \right)^2$$

for $j = 1, \ldots, J$. Here ${}_jx_i$ denotes the number of accidents in subgroup j for site i and ${}_jn_i$ is the monitoring length of that site. Variance and covariance estimates over the subgroups can be found, in the usual way, via

$$\hat{\sigma}_\beta^2 = \frac{1}{J-1} \sum_{j=1}^{J} (\tilde{\beta}_j - \tilde{\beta})^2,$$

$$\hat{\sigma}_\eta^2 = \frac{1}{J-1} \sum_{j=1}^{J} (\tilde{\eta}_j - \tilde{\eta})^2$$

and

$$\hat{\rho} = \frac{\sum_{j=1}^{J} (\tilde{\beta}_j - \tilde{\beta})(\tilde{\eta}_j - \tilde{\eta})}{\sqrt{\sum_{j=1}^{J} (\tilde{\beta}_j - \tilde{\beta})^2 \sum_{j=1}^{J} (\tilde{\eta}_j - \tilde{\eta})^2}}.$$

Repeating the partitioning and averaging estimates may improve the accuracy of the initial parameters.

If the incomplete gamma function is unavailable for the computation of $p_i(v)$, then Bowman and Shenton (1988) describe at least three convenient methods in which this form of $\mathcal{G}(\lambda_i/v \mid s_j, r_j)$ can be numerically computed: expanding the exponential (which converges rapidly if λ_i/v is small); the Stieltjies continued fraction approach; and, the continued fraction of Schlomilch. Moreover, gamma distributed random variates can readily be generated from an algorithm detailed in Fishman (1973) and the 'shoe' variates drawn using the inverse transformation method, as described in Pidd (1986). These methods have been briefly summarised in Appendix D and Section 4.6.3, respectively.

Direct Monte Carlo calculations in each instance, using SAS programming language, were executed using $N = 10,000$. SAS was chosen due to its ability in determining incomplete gamma functions, its random gamma variate generator and SAS has other applicable statistical routines. The standard error of these calculations was in the proximity of ± 0.001, found from multiple recalculations of identical problems and through standard estimation techniques. This degree of accuracy is probably beyond that required by any traffic researcher and $N = 1,000$ could result in more efficient but slightly less reliable estimates.

5.5.2 Case I

We imagine that three sets of responses have been elicited from questions 1 and 2, and are now tabulated in columns 2 and 3 of Table 5.1. As indicated in the discussion pertaining to hyperpriors, we use this information to determine the parameters of the gamma density by the formulae

$$\frac{s_1 + t_1}{2} = \frac{a}{b} \quad \text{and} \quad \left(\frac{t_1 - s_1}{4}\right)^2 = \frac{a}{b^2},$$

a member of the shoe distribution by the formula

$$c = \left(\frac{t_2 - s_2}{4}\right)^2$$

and m is determined by expressing a level of confidence in the practitioner's answer to question 2. This calculation follows easily by observing that $P(0 < \sigma^2 \leq c) = m/(m+1)$, the left hand side of the equation being the degree of confidence in the practitioner's statement about an upper bound on the variance. Note that $h_2(\eta \mid \beta)$ is obtained from (5.6) using the values c and m ascertained above. The results of these computations are contained in columns 4–7 of Table 5.1.

Our first presented criterion for selecting accident sites uses the posterior probability quantity, $p_i(v)$. Based upon three arbitrarily selected v values, $v = 1, 1.1$ and 1.25, the results of this calculation for each of the 35 accident sites are contained in Table 5.2. It is apparent from perusal of Table 5.2 that only the first three sites have any sizeable value for $p_i(v)$. This feature is, perhaps, intuitively implied by the observed data as the observed accident rates for the first three sites are considerably greater than the majority that remain. While intuition suggests that a site with a

Table 5.1: Three hypothetically elicited scenarios from questions 1 and 2.

Scenario	Elicited information		Corresponding hyperparameters			
	(s_1, t_1)	(s_2, t_2)	a	b	c	m
1	(1.00, 3.00)	(0.0, 6.0)	16	8	9/4	4
2	(1.50, 2.50)	(0.5, 4.5)	64	32	1	9
3	(1.75, 2.25)	(0.5, 4.0)	256	128	49/64	19

higher observed accident rate would be more likely to be hazardous than a site with a lower observed accident rate, verification is required to substantiate this intuition. The proposed $p_i(v)$ does this in a very precise quantitative manner.

Table 5.2: Posterior probabilities, $p_i(v)$, for $v = 1, 1.1$ and 1.25.

Scenario	v	Site 1	2	3	4	5	6	7	8	9	...	35
1	1	.495	.238	.239	.005	.021	.000	.001	.001	.000	...	.000
	1.1	.307	.083	.080	.000	.006	.000	.000	.000	.000	...	.000
	1.25	.119	.010	.008	.000	.001	.000	.000	.000	.000	...	.000
2	1	.471	.249	.253	.005	.020	.000	.001	.001	.000	...	.000
	1.1	.283	.086	.086	.000	.006	.000	.000	.000	.000	...	.000
	1.25	.104	.010	.009	.000	.001	.000	.000	.000	.000	...	.000
3	1	.432	.264	.278	.006	.018	.000	.001	.001	.000	...	.000
	1.1	.249	.092	.095	.001	.005	.000	.000	.000	.000	...	.000
	1.25	.084	.011	.010	.000	.001	.000	.000	.000	.000	...	.000
non-info	1	.491	.240	.242	.005	.021	.000	.001	.001	.000	...	.000
	1.1	.304	.083	.081	.000	.006	.000	.000	.000	.000	...	.000
	1.25	.118	.010	.009	.000	.001	.000	.000	.000	.000	...	.000

Table 5.2 illustrates the value of the $p_i(v)$ computation; for example, elicited information corresponding to scenario 1 shows that Site 1 has: a probability 0.495 of having the highest underlying accident rate; a probability of 0.307 that its underlying accident rate is at least 10% larger than the other sites, given by $v = 1.1$; and a probability that decreases to 0.119 for $v = 1.25$. No appreciable differences emerged between the considered information scenarios, including the quasi-noninformative case that is labelled here and thereafter as 'non-info'.

Selection can be made by adopting either of the ensuing approaches. Consider information scenario 2: if (1), with $r = 4$, then clearly Sites 1, 2, 3 and 5 should compose the selected subgroup as these four sites have the largest posterior probabilities; if (2), with probability threshold level $P^* = 0.7$ for $v = 1$, then Sites 1 and 3 should be selected as this subgroup is the smallest with the largest probability of containing the worst site to exceed the threshold value. Should $P^* = 0.99$, however, then Sites 1, 2, 3 and 5 constitute the smallest subgroup to exceed the threshold level.

The second criterion propounded in this thesis uses predictive probabilities, $pd_i(n_0)$'s. Numerical estimates of $pd_i(n_0)$, $i = 1, \ldots, K$, using selected values of n_0, under the three informative scenarios of Table 5.1 and the quasi-noninformative scenario, are summarised for the 35 accident sites in Tables D.1–D.2 contained in Appendix D. Visually instructive summaries of these tables can easily be obtained. One such demonstration is provided in Figure 5.1 for computations assuming information scenario 2.

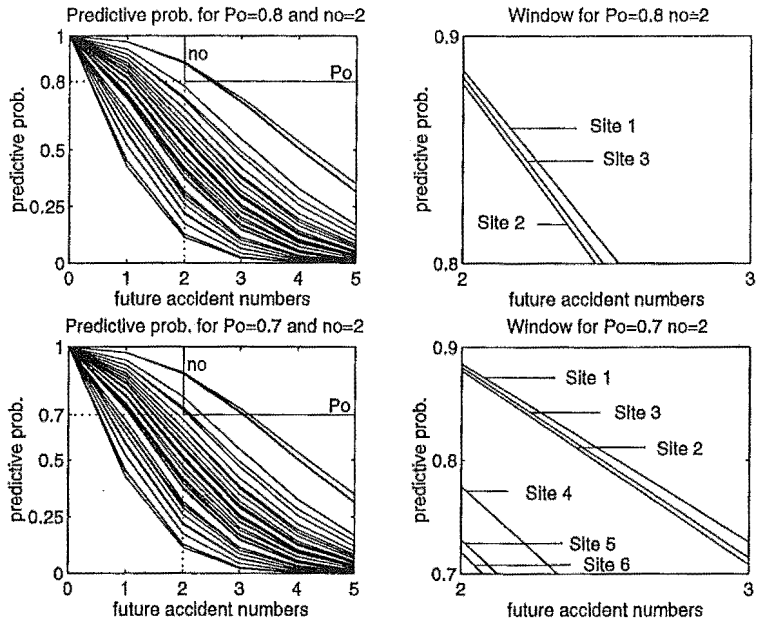

Figure 5.1: Predictive probabilities of future accident numbers, $pd_i(n_0)$, for all 35 sites under scenario 2 hyperprior information and the *selection window* for two (P_0, n_0) combinations.

The left-hand graphs depict the predictive distributions for each of the 35 accident sites, under information scenario 2, and indicates the likelihood that each site exceeds the critical number of accidents n_0, for $n_0 = 0, \ldots, 5$, in the next period.

The practitioner provides a 'window', that is a probability P_0 threshold requirement for a specified hazardous n_0 value. Here, two hypothetical specifications are superimposed upon the left-hand graphs and their respective enlargement constitutes the right-hand graphs in Figure 5.1. Site selection is made by taking those sites that pass through the window. Under the first (P_0, n_0) combination, three sites met the selection criterion (namely, Sites 1, 2 and 3) while under the second (P_0, n_0) combination, six sites are seen to have a predictive probability that exceeds the threshold (namely, Sites 1, 2, 3, 4, 5 and 6). Mathematically, these graphs provide the sites which satisfy the formula

$$P(Y_i > n_0 \mid \boldsymbol{x}) \geq P_0$$

and thereby provides the practitioner with an easily obtained subset of hazardous sites while allowing for various individual requirements to be expressed.

Our third criterion uses posterior means, $\mathrm{E}[\lambda_i \mid \boldsymbol{x}]$, for ranking accident sites. Computed estimates of $\mathrm{E}[\lambda_i \mid \boldsymbol{x}]$ are tabulated in Table 5.3 for the three information scenarios delineated in Table 5.1 and the quasi-noninformative scenario.

Minor differences in estimates across information scenarios are once more evident. Under information scenario 2, hazardous site selection arises from either: (1), for $r = 4$, then Sites 1, 2, 3 and 4 require selection as these four sites have the largest posterior means; or (2), suppose an underlying accident rate of $h = 3.0$ is considered hazardous, then a subgroup containing Sites 1, 2 and 3 should result as no other sites exceed the pre-specified critical value.

From Table 5.3 and depicted in Figure 5.2, for scenario 2, it is noticeable that the range of the posterior means values is considerably smaller than the corresponding range in observed accident rates. It is also noticeable that the ordering of accident sites differs when using the posterior means compared to observed rates. Two factors contribute to these phenomena: sample size; and *shrinkage* (also known as 'regression to the mean' or the 'Stein phenomenon' after Stein (1955) who first published on the inadmissibility of the simultaneous estimation of empirical means).

The hierarchical Bayesian model allows the practitioner to quantify the effect of these factors. If one is comparing a group of accident sites in which some observed rates are based on large samples and some based on small samples, it is to be expected that more variability is inherent within the small samples when compared to large samples, resulting in the small samples being 'shrunk' comparatively more

Table 5.3: Posterior means, $E[\lambda_i \mid \boldsymbol{x}]$, for each prior information scenario.

Site		Scenario			
i	x_i/n_i	1	2	3	non-info
1	4.667	3.968	3.896	3.802	3.958
2	3.875	3.718	3.699	3.673	3.715
3	3.848	3.733	3.719	3.699	3.731
4	3.000	2.902	2.891	2.877	2.899
5	3.000	2.709	2.681	2.650	2.702
6	2.636	2.568	2.561	2.553	2.566
7	2.462	2.376	2.367	2.360	2.372
8	2.333	2.240	2.231	2.227	2.235
9	2.227	2.193	2.190	2.188	2.191
10	2.133	2.096	2.093	2.093	2.093
11	2.000	1.980	1.979	1.982	1.978
12	1.923	1.908	1.908	1.914	1.905
13	1.882	1.875	1.875	1.881	1.872
14	1.867	1.860	1.861	1.867	1.857
15	1.750	1.755	1.757	1.764	1.753
16	1.727	1.740	1.743	1.755	1.736
17	1.684	1.696	1.699	1.707	1.694
18	1.571	1.624	1.632	1.654	1.619
19	1.556	1.601	1.608	1.628	1.597
20	1.500	1.528	1.532	1.544	1.526
21	1.379	1.407	1.411	1.421	1.405
22	1.333	1.451	1.465	1.499	1.446
23	1.313	1.367	1.375	1.393	1.365
24	1.273	1.317	1.324	1.338	1.315
25	1.259	1.297	1.302	1.315	1.295
26	1.059	1.137	1.148	1.170	1.135
27	0.900	1.049	1.068	1.105	1.046
28	0.833	0.971	0.989	1.023	0.968
29	0.833	0.971	0.989	1.023	0.968
30	0.800	1.083	1.114	1.173	1.078
31	0.750	0.866	0.882	0.911	0.864
32	0.714	0.849	0.867	0.900	0.847
33	0.636	0.733	0.746	0.771	0.732
34	0.517	0.600	0.611	0.632	0.599
35	0.421	0.552	0.569	0.601	0.550

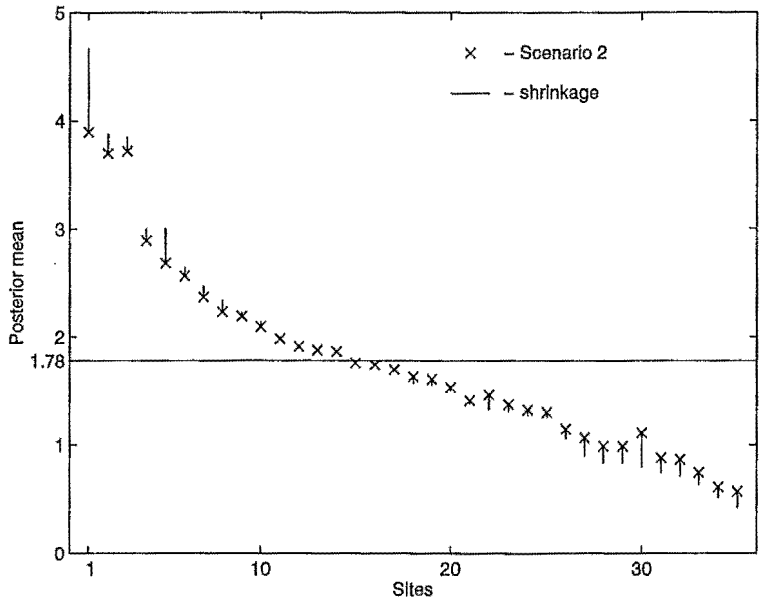

Figure 5.2: Posterior means for the 35 accident sites information scenario 2 (denoted by 'x'), the degree of shrinkage from the x_i/n_i empirical accident rate (denoted by '—') and the pooled accident mean, given by $\sum_{i=1}^{K} x_i / \sum_{i=1}^{K} n_i = 1.78$.

towards the overall group mean. This group mean is some weighted combination of the pooled mean, derived from $\sum_{i=1}^{K} x_i / \sum_{i=1}^{K} n_i$, and the prior mean specified from the elicitation of expert information.

Illustration of this phenomenon is seen clearly in Figure 5.2 with Sites 4 and 5 having the same observed accident rates, yet posterior mean estimates for Site 4, collected over 22 years, shrunk less than Site 5 estimates, which is based on six years of observation. This explains the inversion of ordering between some sites using the posterior mean compared to observed rate orderings and demonstrates very forcefully one of the advantages of the hierarchical model. Albert (1981, 1985) observed a similar phenomenon when simultaneously estimating Poisson means from an empirical and hierarchical Bayesian perspective, respectively. Further comment on these phenomena will be made in Section 5.5.

5.5.3 Case II

It is important to determine whether the specification and embodiment of prior information implies that derived estimates will only be coherent within an associated interval. That is, can an assurance that the estimates be no less than a particular

value or greater than another value for specific prior information be made? The desire to specify bounds arises naturally due to insufficient time, money or resources to elicit specific enough information to draw the assumptions used to specify the hyperprior distributions given by Case I or result from experts who are unable to elaborate further on the population of interest.

So, in this situation, we are interested in providing another interpretation to the answers elicited to questions 1 and 2. We demonstrate that if the broadest interpretation of the elicited information is taken then boundaries associated with any estimate are so widely divergent that the elicited information is of negligible practical use. However, the elicited responses can be interpreted in a variety of ways in order to 'tighten up' the most general interpretation. Here we consider a method, involving some minor additional elicitation, where sensible results can be achieved while still allowing the practitioner considerable flexibility. That is, we provide one method of relaxing the rigid interpretation of questions 1 and 2 presented in Case I so that sensible boundaries around any estimates can be attained.

Broadest interpretation

In Case I, the mean of β was assigned the value $a/b = (t_1 + s_1)/2$. This is now relaxed to simply say that a/b can be anywhere on the (s_1, t_1) interval. Moreover, the variance for β was previously equated to $a/b^2 = [(t_1 - s_1)/4]^2$, but this is now relaxed so that a/b^2 is simply constrained between 0 and its largest possible value, obtained by equally dividing the mass and positioning each half on the boundary points s_1 and t_1 respectively. Remembering that $h_1(\beta) \sim g(\beta \mid a, b)$, then algebraically:

$$s_1 \leq \frac{a}{b} \leq t_1 \quad \Longrightarrow \quad a \geq bs_1 \quad \text{and} \quad a \leq bt_1 \tag{5.18}$$

$$0 \leq \frac{a}{b^2} \leq \left(\frac{t_1 - s_1}{2}\right)^2 \quad \Longrightarrow \quad a \geq 0 \quad \text{and} \quad a \leq \left[\frac{b(t_1 - s_1)}{2}\right]^2. \tag{5.19}$$

Now consider the $h_2(\eta \mid \beta)$ specifications. In Case I, the uniform upper bound before exponential decline on the variability of the λ_i's was equated to $c = [(t_2 - s_2)/4]^2$ and m found on solution to $P(0 \leq \sigma^2 \leq c) = m/(m+1)$, representing the confidence *in* or *of* the practitioner. Suppose now that c can range between the smallest possible variance, equal to 0, and the largest possible variance, again found by placing half the mass on each boundary point s_2 and t_2 respectively. Furthermore, assume

that practitioner confidence can take any realisable positive value of m. Observe that if $m \to \infty$ then σ^2 is uniformly distributed between 0 and c. Algebraically, the relaxation of these constraints implies that

$$0 < m < \infty \quad \text{and} \quad 0 \leq c \leq \left(\frac{t_2 - s_2}{2}\right)^2. \tag{5.20}$$

Under this interpretation, we now investigate the bounds on the selection criteria estimates for information scenario 2 at Site 1. The hypothetical information given by scenario 2 specified $s_1 = 1.5$ and $t_1 = 2.5$. Applying (5.18) gives $a \geq 3b/2$ and $a \leq 5b/2$, and using the variance constraints given by (5.19), then $a \geq 0$ and $a \leq b^2/4$. Similarly, noting that $s_2 = 0.5$ and $t_2 = 4.5$, and recalling (5.20), then it follows that $0 \leq c \leq 4$.

The maximum values of each selection criteria function for Site 1 occur when $a \to \infty$ and $b \to \infty$ on the line $a = 5b/2$, effectively implying that $\beta = 5/2$, together with $m \to 0$ and $c = 4$. Results for the selection criteria using these parameter values are included in Table 5.4.

Table 5.4: Broadest boundary selection criteria estimates (min, max) for Site 1 assuming information scenario 2 and values of $p_i(v)$, $i = 2, \ldots, 35$ and $v = 1, 1.1, 1.25$, under the situation where the minima and maxima of $p_1(v)$ are computed.

Site	$p_i(1)$	$p_i(1.1)$	$p_i(1.25)$
1	(0.000, 0.623)	(0.000, 0.434)	(0.000, 0.203)
2	(0.000, 0.180)	(0.000, 0.060)	(0.000, 0.007)
3	(0.000, 0.160)	(0.000, 0.047)	(0.000, 0.004)
4	(0.000, 0.004)	(0.000, 0.000)	(0.000, 0.000)
5	(0.000, 0.031)	(0.000, 0.011)	(0.000, 0.002)
6	(0.000, 0.000)	(0.000, 0.000)	(0.000, 0.000)
7	(0.000, 0.001)	(0.000, 0.000)	(0.000, 0.000)
8	(0.000, 0.001)	(0.000, 0.000)	(0.000, 0.000)
9	(0.000, 0.000)	(0.000, 0.000)	(0.000, 0.000)
⋮	⋮	⋮	⋮
35	(0.000, 0.000)	(0.000, 0.000)	(0.000, 0.000)

$pd_1(1)$	$pd_1(2)$	$pd_1(3)$	$pd_1(4)$	$pd_1(5)$
(0.838, 0.983)	(0.545, 0.917)	(0.279, 0.788)	(0.116, 0.615)	(0.040, 0.434)

$\mathrm{E}[\lambda_1 \mid \boldsymbol{x}]$
(1.833, 4.347)

Minimisation of the criteria for Site 1 occurs when $a \to \infty$ and $b \to \infty$ on the line

$a = 3b/2$, implying that $\beta = 3/2$, together with $m \to \infty$ and $c \to 0$, implying that $\eta = 0$ with probability one. Results using these parameter values are also included in Table 5.4. Under this specification of parameters it is evident that, $\mathrm{E}[\lambda_i \mid \boldsymbol{x}] = 3/2$, $Var(\lambda_i \mid \boldsymbol{x}) = 0$ and hence $p_i(v) = 0$ for all $i = 1, \ldots, 35$ and $v \geq 1$, no matter what data are observed. Moreover, in this limit $\sum_{i=1}^{35} p_i(1) \neq 1$, which is contrary to that expected when summing posterior probabilities over all sites for $v = 1$. These features are clearly unsatisfactory from a practical point of view. In the following section we address this difficulty.

More sensible boundary specifications

To compensate for the inadequacies wrought by the broadest interpretation discussed above, we require added information to that formerly elicited from questions 1 and 2. Specifically, in addition to the responses for question 1, the practitioner needs to state an interval for the probability, p, that the average accident rate is contained within the interval (s_1, t_1). For convenience we assume the probability that the average accident rate is below s_1 is equal to the probability that the average accident rate is above t_2, with value $(1-p)/2$. This information restricts the bounds for (a, b) from those used in the preceding section.

Next, instead of allowing (c, m) to range over the parameter space given by question 2 and (5.20), we constrain these parameters to a smaller domain by using intervals of uncertainty. For a fixed c (derived using the methods of Case I, say) we allow $\underline{q} \leq P(0 \leq \sigma^2 \leq c) \leq \overline{q}$, for some probability interval $(\underline{q}, \overline{q})$, to describe the confidence of the practitioner that $\sigma^2 < c$. This implies that $\underline{q} \leq m/(m+1) \leq \overline{q}$, and defines appropriate bounds for m. A simple construction for the c-interval assigns $\underline{c} = c - c/2$ and $\overline{c} = c + c/2$. There are apparent modifications to both of these approaches which are being investigated further. With this supplementary information we are able to deduce allowable families $\mathcal{h}_1(\beta)$ and $\mathcal{h}_2(\eta \mid \beta)$ for the respective hyperpriors $h_1(\beta)$ and $h_2(\eta \mid \beta)$. The mathematical details of this now follow.

Derivations of $\mathcal{h}_1(\beta)$

We require the practitioner to specify an interval, say $(\underline{p}, \overline{p})$, for the probability p that the average accident rate is within the interval (s_1, t_1). Here we assume the

probability that this average is below s_1 is equal to the probability it is above t_1 with value $(1-p)/2$. These constraints result in the $h_1(\beta)$ distribution, $g(\beta \mid a, b)$, having parameters a and b that must lie on the solid curve indicated in Figure 5.3.

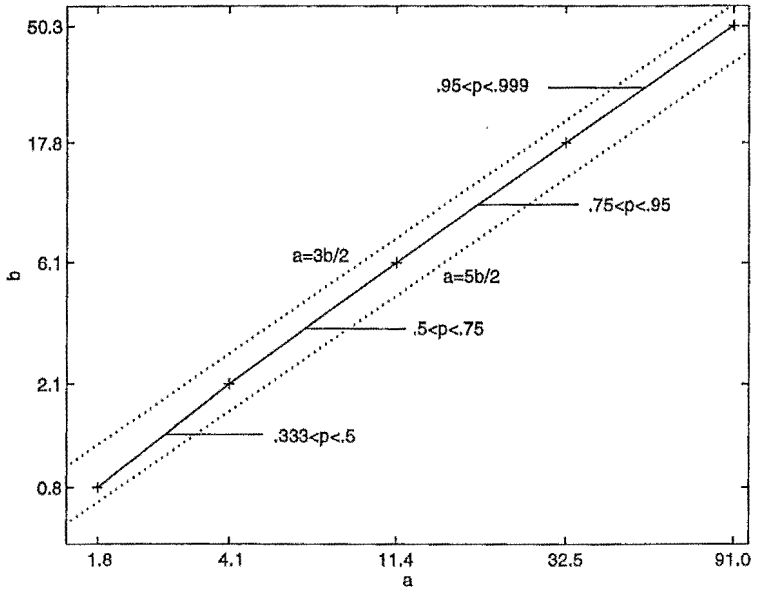

Figure 5.3: A log-scaled plot of valid (a, b) combinations for elicited p–intervals under scenario 2 hyperprior information.

Some selected interval values for $(\underline{p}, \overline{p})$ appear in Figure 5.3; for example if $(\underline{p} = 0.5, \overline{p} = 0.75)$ then the (a, b) parameters consistent with this information lie on the solid curve between (4.1, 2.1) and (11.4, 6.1). Also depicted in this figure are the boundaries corresponding to information scenario 2 which stipulated that $(s_1 = 1.5, t_1 = 2.5)$ and hence implied $a \geq 3b/2$ and $a \leq 5b/2$. From Figure 5.3 it is evident that any specified $\underline{p}$ above 0.333 is coherent with the response provided to question 1. It is also clear that there exist potential instances where the intervals expressed for p and the values elicited for (s_1, t_1) are inconsistent. The exact value where p is no longer coherent was not explicitly found as it was not relevant to the example.

Derivations of $h_2(\eta \mid \beta)$

Initially we determine a family on the distribution for σ^2 and then use the transformation $\sigma^2 = \eta\beta$ to deduce a family of allowable hyperpriors for $h_2(\eta \mid \beta)$.

In Case I, elicitation of question 2 and our interpretation of that information

enabled the specification of a bound c on the variance σ^2. To allow for some measure of mis-specification, we assigned a positive probability that σ^2 could be larger than that c, and this defined the shoe distribution with parameters c and m. In the Case II scenario, c will no longer be fixed but rather have an interval $(\underline{c}, \overline{c})$. A simple construction of this interval, taken in this thesis, assigns $c = (t_2 - s_2)^2/16$ (as in Case I) and then takes $\underline{c} = c - c/2$ and $\overline{c} = c + c/2$. This interval was chosen for convenience; there are apparent modifications to this approach.

Previously, in Case I, m was chosen so that $P(0 \leq \sigma^2 \leq c) = m/(m+1)$. We now express our confidence in or of the practitioner about the bound on the variance, c, with a probability interval $(\underline{q}, \overline{q})$ so that $\underline{q} \leq P(0 \leq \sigma^2 \leq c) \leq \overline{q}$. For m to be consistent with this interval, it must satisfy the inequalities given by $\underline{q} \leq m/(m+1) \leq \overline{q}$.

These intervals define the regions where values of (c, m) must lie to be consistent with the elicited information. Supposing confidence in the practitioner, for

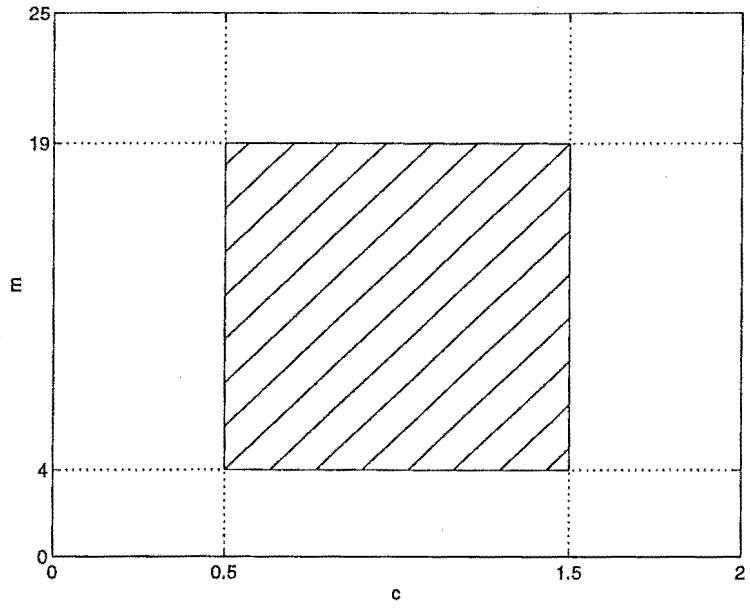

Figure 5.4: The shaded region provides valid (c, m) combinations associated with information specified by the intervals $0.80 \leq P(0 \leq \sigma^2 \leq c) \leq 0.95$ and $0.5 \leq c \leq 1.5$.

prior information expressed by scenario 2, was assigned the probability interval $0.80 \leq P(0 \leq \sigma^2 \leq c = 1) \leq 0.95$ then the family $h_2(\eta \mid \beta)$ of parameters consistent with the elicited responses are graphically presented in Figure 5.4. A shoe distribution consistent with this information can have any c and m value contained within

the shaded bounded region.

The search for maximum and minimum values for each of the selection criteria were restricted to those hyperparameters consistent with the elicited information and contained in allowable families $h_1(\beta)$ and $h_2(\eta \mid \beta)$.

Maximum and minimum values for each of the criteria functions over families $h_1(\beta)$ and $h_2(\eta \mid \beta)$ can now be obtained. Results for Site 1 using selected hypothetical intervals on p, based upon $0.80 \leq P(0 \leq \sigma^2 \leq c) \leq 0.95$ and $0.5 \leq c \leq 1.5$, are reported in Table 5.5 (again, values for $p_i(v)$, $i = 2, \ldots, 35$, under this prior specification are included for comparison).

Table 5.5: Tightened boundary selection criteria estimates (min, max) for site 1 assuming information scenario 2 and values of $p_i(1)$, $i = 2, \ldots, 35$, under the situation where the minima and maxima of $p_1(1)$ are computed.

Selection	p–interval			
criteria	0.95 – 0.999	0.75 – 0.95	0.5 – 0.75	0.333 – 0.5
$p_1(1)$	(0.424, 0.470)	(0.424, 0.470)	(0.425, 0.471)	(0.426, 0.473)
$p_2(1)$	(0.267, 0.249)	(0.267, 0.249)	(0.267, 0.249)	(0.266, 0.247)
$p_3(1)$	(0.285, 0.254)	(0.285, 0.254)	(0.284, 0.254)	(0.283, 0.253)
$p_4(1)$	(0.006, 0.005)	(0.006, 0.005)	(0.006, 0.005)	(0.006, 0.005)
$p_5(1)$	(0.017, 0.019)	(0.017, 0.019)	(0.017, 0.019)	(0.017, 0.020)
$p_6(1)$	(0.000, 0.000)	(0.000, 0.000)	(0.000, 0.000)	(0.000, 0.000)
$p_7(1)$	(0.001, 0.001)	(0.001, 0.001)	(0.001, 0.001)	(0.001, 0.001)
$p_8(1)$	(0.001, 0.001)	(0.001, 0.001)	(0.001, 0.001)	(0.001, 0.001)
$p_9(1)$	(0.000, 0.000)	(0.000, 0.000)	(0.000, 0.000)	(0.000, 0.000)
$\vdots$	$\vdots$	$\vdots$	$\vdots$	$\vdots$
$p_{35}(1)$	(0.000, 0.000)	(0.000, 0.000)	(0.000, 0.000)	(0.000, 0.000)
$pd_1(1)$	(0.972, 0.975)	(0.972, 0.975)	(0.972, 0.975)	(0.972, 0.975)
$pd_1(2)$	(0.876, 0.886)	(0.876, 0.886)	(0.876, 0.887)	(0.877, 0.887)
$pd_1(3)$	(0.710, 0.729)	(0.710, 0.729)	(0.711, 0.729)	(0.712, 0.730)
$pd_1(4)$	(0.513, 0.536)	(0.513, 0.536)	(0.513, 0.536)	(0.514, 0.538)
$pd_1(5)$	(0.330, 0.353)	(0.330, 0.353)	(0.331, 0.353)	(0.331, 0.354)
$\mathrm{E}[\lambda_1 \mid \boldsymbol{x}]$	(3.780, 3.901)	(3.780, 3.901)	(3.782, 3.903)	(3.785, 3.906)

From Table 5.5, derived using information scenario 2 and further elicitation, the range between maximum and minimum values for each selection criteria estimates are much smaller than Table 5.4. These tightened intervals gives the practitioner more confidence in the estimates for each of the ascertained criteria despite the

uncertainty inherent within the elicited information, and illustrates the value of extra information from responses to questions 1 and 2.

Chapter 6

Summary

We now recapitulate both the proposed techniques and the main findings from the application of these techniques to the Auckland data.

6.1 Model discrimination

6.1.1 Averaged Bayes Factor

When selecting between a multiple of mathematical models (each having a vector of unknown parameters) at a collection of sites, it is unlikely that sufficient expert subjective knowledge will always be available to create proper prior distributions so that standard informative Bayesian analyses can proceed. In these instances, utilisation of noninformative priors provides a realistic and feasible tool for analysts to discriminate between models in the Bayesian framework. Implementation of such priors have traditionally has been fraught with difficulties due to the arbitrary nature of the multiplicative constant. Adoption of training samples provides a method of resolution, thereby facilitating a powerful noninformative Bayesian selection mechanism.

In this thesis we introduced the *averaged Bayes factor*. This technique assures coherent pairwise model comparisons and facilitates posterior probability derivations

useful for simultaneous model discrimination and selection. The averaged Bayes factor method also produces quantitative, computationally straightforward and interpretable answers. Moreover, due to the averaging process, this method provides stable answers that are independent from particular training samples. Not all these properties are shared by existing noninformative Bayesian methods. Additionally, the averaged Bayes factor facilitates selection between competing models whether nested, nonnested or some combination. The latter is achieved only with considerable effort in the non-Bayesian framework, particularly with such small sample numbers.

We have demonstrated that in the traffic accident analysis context, model selection using the BIC criterion favours, often quite substantially, the simpler models when compared to the averaged Bayes factor approach. This failing was clearly illustrated by the Poisson model (M_1), and to a lesser extent the geometric model (M_4), having considerably more support under the approximated BIC selection method than under the corresponding comparisons using averaged Bayes factors. The deficiency of the BIC method is due to its asymptotic development whereby a term is justifiably ignored as the sample size tends to infinity. Unfortunately, when the sample size is relatively small, this ignored term can impact significantly on the resultant Bayes factor and its omission creates a substantial systematic bias. Typically, traffic accident analysis deals with small sample sizes, thereby introducing potentially serious bias into the BIC selection procedure or its approximations.

From the properties given in Section 3.2 and on the basis of the numerical example, it seems that the averaged Bayes factor method has wider applicability than many of its competitors.

6.1.2 Application of the averaged Bayes factor

Applying the averaged Bayes factor on the Auckland data included in Table A.1 we demonstrated that the Poisson model was the most frequently favoured of those considered. Also apparent was the consistency in the favourability of the Poisson/gamma model; this model never having a discrimination rank below two of the four models considered over the 35 accident sites. This consistency accounted for the averaged posterior probabilities for both the Poisson and Poisson/gamma models being almost identical with $\overline{P}(M_1 \mid \boldsymbol{x}) = 0.313$ and $\overline{P}(M_2 \mid \boldsymbol{x}) = 0.309$.

Without model adequacy considerations, the weight of support, at this stage, would probably favour the Poisson model. The appeal of its simplicity coupled with its discrimination ranking and $\overline{P}(M_1 \mid \underline{x})$ probability superiority over the other models would suggest that accident analysis should precede with the adoption of this model.

Similarly, without verification of the Poisson model's adequacy, it would have undoubtedly been selected as the most appropriate to best represent the hypothetical, binomial generated, Site B data. This discrimination on data deliberately chosen to be discordant from all the candidate models forcefully demonstrates the inadequacies of the Bayes factor approach if used alone for model selection purposes.

6.2 Model adequacy and Power

6.2.1 Remarks

It is clear that model selection and model adequacy are interrelated but neither implies the other. We believe, therefore, that upon selection it is important to directly investigate the likelihood of observed data originating from the chosen model. If data and their associated selected model are irreconcilable then it is unlikely that any ensuing inferences based on this inadequate model will be accurate or useful. In such circumstances it may be appropriate to extend the set of candidate models available for model selection or re-examine the data. If, however, the inadequate model is utilised then considerable care must be taken over the interpretation of any results.

Model adequacy does not imply model selection as frequently many different models, of varying degrees of complexity and dimension, exist or can be constructed that are consistent with some data under analysis. Highly sophisticated or overly specified models are infrequently the most parsimonious and rarely appropriate. Good model selection techniques, such as the Bayes factor approach, discriminate between competing models based on their complexity and comparative likelihood. We thus concur with Upadhyahy and Smith (1993) and do not advocate adequacy as a method for model selection, instead we view model adequacy as a method providing guidance as to whether a particular discriminated model seems compatible with the

observed data.

In this thesis we describe an intuitive method that enables both model adequacy and its associated power to be quantifiably and sensibly ascertained, using methods in cross-validation, prediction and simulation. The proposed simulation scheme delineated within allows the construction of pictorial representations of these entities to be easily undertaken thereby allowing a fuller understanding of the relationship between data and selected models to be derived.

We believe that it is important for model adequacy to be recognised and addressed once mathematical representations of the data have been selected. If adequacy is ignored, how can any researcher have confidence in their ensuing analyses and inferences?

6.2.2 Adequacy measures

Model adequacy was conducted using three separate $\mathcal{D}^r$ measures. Generally, the most powerful and robust of these considered measures was $\mathcal{D}^1$, the chi-square measure. The applicability of this measure depends, however, on the availability of the mean and variance of the hold-out predictive distribution. In their absence, pseudo-values allowed the adoption of the $\mathcal{D}^1$ measure. Results from this $\mathcal{D}^1$ adaptation performed satisfactorily and with reasonable power for the examples demonstrated within this thesis. However, the general applicability and suitability of this measure estimated using these contrived pseudo-entities certainly requires further investigation. Nonetheless, based upon the results contained in this thesis, we recommend $\mathcal{D}^1$ as the most suitable measurement of discrepancy although further confirmation using a greater breadth of distributions, adequacy measures and data is required.

Adequacy measured by $\mathcal{D}^3$ was invariably less powerful than corresponding $\mathcal{D}^1$ measures. However, the $\mathcal{D}^3$ measure is attractive in the sense that it was unrestricted by the indefinite mean and variance quantities that compromised the $\mathcal{D}^1$ measure. This adequacy measure, therefore, is a suitable and appropriate companion to the $\mathcal{D}^1$ measure.

It was surprising to find that the $\mathcal{D}^2$ measures were widely inconsistent in their power. As a consequence of the extremely poor power frequently associated with the $\mathcal{D}^2$ measure under certain conditions, we can not recommend $\mathcal{D}^2$ as a useful global adequacy measure.

6.2.3 Application

It was clearly demonstrated that the 'best' model, in the discriminatory sense, is not necessarily adequate. All the considered measures resoundingly rejected the applicability of the Poisson model on the hypothetical accident Site B. In was evident the Poisson model was patently deficient in modelling the under-dispersion associated with this site. Ensuing analyses using this best model would almost certainly result in erroneous or misleading conclusions.

When examining the 35 accident sites collectively, the inconsistent global adequacy of the Poisson model comparative to the Poisson/gamma model became apparent. Using the powerful $\mathcal{D}^1$ adequacy measure, at eight sites (23%) the Poisson model was deemed inadequate at $\alpha = 0.05$ while the Poisson/gamma model recorded two (6%) such inadequacies. The model inadequacy frequency that was associated with the Poisson density casts serious doubt on its global applicability, especially since the Poisson/gamma model performs so comparatively well. This result may appear quite discrepant or contrary from that anticipated after the discriminatory success of the Poisson model. However, an explanation for this result can be provided using the following reasoning.

To understand this phenomenon we first need to revisit the averaged Bayes factor results. The natural embodiment of Occam's razor within the Bayes factor calculations ensures that the Poisson model is always favoured over the Poisson/gamma model (which has larger dimensionality) when the data have empirical dispersion index close to one. Despite this, the Poisson/gamma is usually only *minimally* worse than the Poisson model on these occasions. However, in the presence of over-dispersed data, the favourability of the Poisson model falls away relatively quickly and the preference of the Poisson/gamma model is revealed. In these instances the Poisson frequently slipped to the fourth and worst rank, and was typically *very strongly* worse than the Poisson/gamma model. Consequently, as a model, the Poisson model is quite extreme, in the sense that: when it is best, it is good; but when it is worst, it is terrible! By comparison, the Poisson/gamma model is far more circumspect and accommodating.

With the simultaneous ranking and selection between hazardous accident sites, it thus appears that the Poisson/gamma more appropriately accommodates the diversity inherent within accident data. Further research conducted on accident

data sets from alternative sources is required before this recommendation can be offered with more certainty.

6.3 Ranking and selection

The analyses of Section 5.5 illustrates quite forcefully the advantages and salient features of the hierarchical model and corresponding selection criteria proposed in this thesis. These ideas are explained below.

6.3.1 Hierarchical model

Among the basic facts that motivate this analytical technique is that in many multivariate estimation problems, such as those encompassed in vehicle accident studies, the 'standard' maximum likelihood estimates employed are inadmissible, there is no facility to incorporate the often abundant subjective information concerning the accidents sites, and standard tests of hypothesis invariably provide unsatisfactory non-significant results due to large associated standard errors. These deficiencies can be surmounted by embracing a hierarchical Bayesian paradigm.

A distinguishing trait of the hierarchical model, then, is its ability to quantitatively, accurately and easily discriminate between sites that commonly have small and variable accident count periods. In particular, the model naturally discriminates between sites (without any special considerations) when observed accident rates from q sites, $q \leq K$, are equal while the period of monitoring is in fact different. For example from Table 5.3 it can be seen that the observed accident rate for both Sites 4 and 5 is 3.0, however, when using a noninformative hyperprior and $v = 1$, it can be seen from Table 5.2 that the posterior probability that Site 5 is worst is 4.2 times more likely than Site 4. This discrepancy in posterior probabilities is due to the differing length of observation periods; here Site 4 had data recorded over 22 years while Site 5 was recorded over six years.

When adopting the noninformative hyperprior and $v = 1$, the posterior probability of obtaining the worst accident rate equalled 0.973 for the subgroup composed of Sites 1, 2 and 3. Instead, if $r = 4$, then the best subset contains Sites 1, 2, 3 and 5 with an associated posterior probability of 0.994. On this basis, should reconstruction of Sites 1, 2, 3 and 5 be undertaken then the probability that the

worst accident site remains unselected is 0.006. Notice that Site 4 is not selected here although it has the same observed accident rate as Site 5 (which is selected).

The hierarchical model provides a natural mechanism whereby prior information can be elicited and incorporated in the analysis. The hypothetical answers we used in Section 5.5 illustrate the way in which the practical information can be useful in the analysis. The model itself shows how this information is to be used. This type of decision making has not been available to practising engineers in other kinds of analyses.

6.3.2 Selection criteria

The three selection criteria suggested in this thesis have been shown to offer a variety of useful information when applied to the data in Table A.1. The various characteristics of these criteria indicate when they should be appropriately employed. Using the $p_i(v)$ allows the practitioner the ability to determine which site has the highest underlying accident rate and by how much. The $pd_i(n_0)$ criterion, on the other hand, offers a different but equally valid method of selecting hazardous sites based upon the number of accidents in the next period. Finally, the third criterion, that of the mean underlying accident rate of a site, offers other insights into ranking sites for remedial treatment.

Generally the three criteria do agree in their ranking but there are some minor differences. For example, when using the $pd_i(n_0)$ criterion for Sites 20, 21 and 22 then: for $n_0 = 1$, Sites 20 and 21 are preferred over Site 22; for $n_0 = 2, 3$ and 4, Site 20 is preferred over Site 22 which in turn is preferred over Site 21; and for $n_0 = 5$, Site 22 is preferred over both Sites 20 and 21 (although not reported here, the latter is also true for $n_0 > 5$). Similarly, under all considered hyperprior scenarios $\mathrm{E}[\lambda_5 \mid \boldsymbol{x}] < \mathrm{E}[\lambda_4 \mid \boldsymbol{x}]$ while $p_5(v) > p_4(v)$. Other differences are evident but remain minor.

Case I results were quite insensitive to the four quite disparate hypothetical information scenarios employed. The robustness of the estimates gives confidence in both the model employed and the data themselves. Furthermore, meaningful estimator boundaries were achieved, as demonstrated by Case II analyses, with the elicitation of additional information to question 1. These boundaries give the practitioner a grasp of the potential variation associated with the selection criteria

estimates, and a confidence band in which estimators are most likely to be found.

The current focus on identifying the worst locations is based on the premise that once a location has been identified, diagnosis of the problems and potential treatments will be straightforward (that is the deficiencies and remedies will be obvious to an experienced accident investigator). It was from this perspective that selection was introduced and demonstrated in this thesis. Consideration should be given to the identification of best locations (those locations with the lowest underlying accident rates) as examination of these sites and comparison with worst sites may well assist identification of differences in the two types of locations and suggest appropriate treatments for the worst locations (to make them more like the best locations). Ranking and selection of the best locations can be easily attained using any of the selection criteria suggested within this thesis simply through the reversal of the inequality sign in (5.13), (5.15) and all subsequent respective equations.

6.4 General extensions

6.4.1 Averaged Bayes factor

As previously alluded to, model discrimination in the traffic accident analysis framework typically deals with small sample sizes. Such diminutive samples allow individual observations to have a substantial influence on the averaged Bayes factor, or any Bayes factor variant for that matter. A diagnostic, such as that proposed by Pettit and Young (1990), can easily be developed to detect an observation which is most influential on the averaged Bayes factor. This diagnostic would provide more insight into both the data (so that seemingly peculiar observations could be identified and verified from their source or record) and the models under comparison.

There are a plethora of model discrimination techniques available, of which the averaged Bayes factor is but one. However, the desirable properties and intuitive derivation associated with this technique (Section 3.2) suggests that its applicability should be further investigated on a more diverse array of problems, such as providing regression diagnostics.

6.4.2 Model adequacy

Although not explicitly considered here, model adequacy can be further extended to determine whether elicited and modelled informative prior densities combined with some assumed (or selected) likelihood function are consistent with the observed phenomena $\boldsymbol{x}$. Adequacy calculations of this type could usefully assess and validate the reliability of any prior information.

We note that the full Bayesian paradigm has not been applied to the proposed model adequacy stratagem. That is, in accordance with the Bayesian philosophy, the uncertainty about the adequacy of a model should ideally be described by a probability distribution. This area is open for further development.

6.4.3 Bayesian hypothesis testing

Although this is generally not the definitive objective of a traffic engineer, there may be instances where testing the equivalence of unknown accident rates between sites is necessary. An alternative model for significance testing within a Bayesian framework, initiated by Jeffreys (1967) and continued by Deely and Gupta (1988), can be applied to test $\mathrm{H}_0 : \lambda_1 = \lambda_2 = \ldots = \lambda_K$. Mathematical details now follow.

Recall that the prior distribution (5.2) has mean and variance $\mathrm{E}[\lambda_i \mid \beta, \eta] = \beta$ and $Var(\lambda_i \mid \beta, \eta) = \eta\beta$, see (5.4), so by incorporating a prior probability γ that H_0 is true it is straightforward to develop a significance test. That is, a value γ is assigned so that $P(\mathrm{H}_0 \text{ is true}) = P(\eta = 0) = \gamma$. The posterior probability of H_0 is found by computing

$$\gamma^* = \left[1 + \frac{1-\gamma}{\gamma}\frac{f(\boldsymbol{x})}{f(\boldsymbol{x} \mid 0)}\right]^{-1}$$

where $f(\boldsymbol{x})$ and $f(\boldsymbol{x} \mid \beta, \eta)$ are given by (5.9) and (5.8) respectively, thus

$$\begin{aligned} f(\boldsymbol{x} \mid 0) &= \int_0^\infty f(\boldsymbol{x} \mid \beta, 0)\, h(\beta, 0)\, d\beta \\ &= \int_0^\infty \prod_{i=1}^{k} \left[\frac{1}{x_i!}\right] \beta^{k\bar{x}} e^{-k\beta} h(\beta, 0)\, d\beta \end{aligned}$$

where $\bar{x} = \sum_{i=1}^{k} x_i/k$. Each $p_i(v)$ should be multiplied by $(1-\gamma^*)$ to obtain the posterior probability that λ_i is largest since $p_i(v)$ is conditional upon H_0 being false; which implies $\eta > 0$.

6.4.4 Countermeasure evaluation

The evaluation of accident countermeasures and the identification and ranking of hazardous locations can be reduced to a before and after study. That is, one is interested in ascertaining whether some treatment is effective in reducing the underlying accident rate for a given site. Although not specifically considered in this thesis, it follows directly that the hierarchical Bayesian framework can easily be applied to this situation. Treating the series of accidents before and after the accident site reconstruction separately, placing prior distributions and combining with the observed accident frequencies, the posterior distribution can be constructed. The selection criteria can then be utilised to evaluate the effectiveness of the reconstruction on reducing the underlying accident rate.

6.4.5 Cost and loss

Implicated in the selection criteria and ensuing selection strategies has been the notion of equivalence between accident sites in terms of cost, C, of intervention and potential for accident reduction. Although not detailed here, these selection ideas can be extented to situations where this equivalence no longer exists, so that $C_i \neq C_j$ for sites i and j respectively.

The posterior probability selection criteria suggested in this thesis inherently incorporates an analogue of the "0–K" *loss function* (see Berger, 1985, for example). Loss is zero if a correct decision is made (selection of a hazardous site or omission of a non-hazardous site), and K if an incorrect decision made (selection of a non-hazardous site or omission of a hazardous site). Selection based upon the proposed $p_i(v)$ probabilities ensures the minimised expected loss. This loss function can be extended to situations where actions at different sites incur different losses.

6.4.6 Hierarchical Bayesian modifications

There are various modifications of the hierarchical model that might be explored. Firstly, a general linear model as considered in Christiansen, Morris and Pendleton (1992) may give some improved accuracy. For example, the replacement of β in (5.2) by $y_{i1}\beta_1 + y_{i2}\beta_2 + \ldots + y_{iq}\beta_q$ where $y_{i1}, y_{i2}, \ldots, y_{iq}$ are known 'regressors' for $i = 1, \ldots, k$ and $\boldsymbol{\beta} = (\beta_1, \beta_2, \ldots, \beta_q)$ is a vector of unknown 'regression' coefficients

with hyperprior $h_1(\beta)$. This model would incorporate various descriptions of changes in λ_i as well as the naive Bayesian model in which each λ_i is assumed independent with a known gamma distribution but with possibly different parameters.

Another possible extension of the hierarchical Bayesian model involves the notion of partial exchangeability (de Finetti, 1974, Diaconis 1988, Lad 1996), particularly relevant when K is large. This thesis has concentrated on the situation where K is moderately small and homogeneous, assuming all K sites are exchangeable. In some instances exchangeability amongst an entire group of sites may not be realistic, instead exchangeability may be tenable only within subgroups and from subgroup to subgroup exchangeability may only exist in their means. This fact may not be recognisable until after observing the data, however the hierarchical Bayesian model should be enriched to allow this possibility of partial exchangeability.

6.5 Final remarks

If one is to properly understand traffic accidents, more must be learnt about their behaviour; and that if one expects to control traffic accident occurrence efficiently and provide suitable means for control, one must be able to uniformly estimate and predict traffic accident patterns. Only when efficient statistical methods are implemented will traffic management arrive at rules of action that best address accident reduction, and minimise the enormous cost to society. It is hoped that the statistical techniques presented in this thesis make some advancement in that direction.

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Appendix A

Auckland data

To illustrate the strategies introduced in this thesis we use data obtained from 35 traffic intersection sites in Auckland city, along with information about changes in intersection layout or form of control. The most recent series were taken such that no series bridged a change in intersection layout or control. These data have been previously reported in published literature by Nicholson (1985) and are included in Table A.1 below. The series duration ranged from five to 33 years inclusively, with a 16 year median.

In addition, for illustrative purposes, we include some hypothetical accident data generated from a binomial $\mathcal{B}(n = 5, p = \frac{1}{2})$ model. This particular binomial specification, with $\mathrm{E}[x] = 5/2$ and $Var(x) = 5/4$, was deliberately chosen so that generated data would have an empirical mean resembling the more hazardous sites in Table A.1 while having considerably less variability. Although numerically convenient, this particular binomial parameter specification has little contextual meaning as "n" usually corresponds the number of trials and "p" represents the probability of an event. The annual traffic count entering each of these 35 sites has been estimated to be in the vicinity of eleven million (Auckland City Council, 1996) thence the probability of an accident is extremely small.

The hypothetical accident site will be referred to as Site B.

Table A.1: Annual traffic accident counts for 35 intersection sites in Auckland, New Zealand, and one hypothetical site labelled Site B.

Site	n	Observed annual accident counts
1	6	2,3,3,4,9,7
2	24	1,4,4,6,8,2,6,5,7,4,4,6,5,3,6,3,3,5,3,5,1,1,0,1
3	33	2,3,2,2,3,2,3,1,2,2,4,4,6,4,10,9,6,6,10,4,5,5,4,4,3,4,6,5,3,2,1,0,0
4	22	2,2,2,2,3,2,5,5,2,2,3,4,7,6,7,1,5,3,1,0,1,1
5	6	5,2,2,3,5,1
6	22	4,2,2,2,3,5,5,2,3,3,3,3,1,3,2,3,3,1,3,2,2,1
7	13	1,1,1,1,4,5,2,3,3,5,1,1,4
8	9	1,1,0,1,3,2,4,5,4
9	22	1,1,2,3,1,5,5,4,0,2,3,5,1,1,7,4,1,1,0,0,1,1
10	15	6,11,2,4,0,1,1,1,2,0,0,2,1,1,0
11	17	3,2,0,2,2,1,2,1,4,3,6,1,2,1,1,0,3
12	13	1,3,1,1,1,2,2,4,5,1,0,1,3
13	17	0,1,3,4,2,7,4,3,2,1,0,0,2,2,0,0,1
14	15	3,4,2,3,2,0,3,0,1,3,1,3,2,0,1
15	20	0,0,2,0,1,1,0,0,2,3,3,2,2,5,2,2,2,3,1,4
16	11	1,3,1,0,1,2,3,0,2,2,4
17	19	0,3,2,1,1,1,2,2,4,3,1,1,1,2,2,3,1,1,1
18	7	6,2,1,1,0,0,1
19	9	4,2,1,2,0,1,1,0,3
20	20	0,2,0,2,2,1,2,1,2,1,1,3,1,4,0,2,3,1,2,0
21	29	2,2,2,1,0,2,1,2,1,3,1,0,0,0,0,4,3,1,1,0,3,0,1,0,1,1,1,3,4
22	6	3,0,1,2,1,1
23	16	3,0,3,1,0,1,2,0,6,0,0,1,2,0,1,1
24	22	2,0,0,0,1,0,0,2,1,2,4,0,3,0,2,1,1,2,1,0,3,3
25	27	0,0,0,0,1,1,1,1,2,0,1,0,2,0,3,3,2,0,5,3,0,3,1,1,1,1,2
26	17	1,0,0,0,1,0,1,2,4,1,1,1,1,0,2,2,1
27	10	2,0,1,0,2,2,1,0,0,1
28	12	0,1,1,2,1,0,0,0,1,1,2,1
29	12	2,1,0,1,0,1,0,0,3,1,0,1
30	5	1,1,0,1,1
31	16	2,5,0,0,2,1,0,0,0,0,0,2,0,0,0,0
32	14	0,0,1,0,0,3,2,0,2,0,0,0,0,2
33	22	0,2,3,0,1,1,0,0,2,0,0,0,0,2,0,1,0,1,0,0,1,0
34	29	0,0,1,0,0,1,0,0,0,1,0,2,0,0,0,1,1,1,0,0,0,0,0,0,2,1,0,2,0,2
35	19	0,0,0,0,0,2,0,0,1,0,0,2,1,0,0,1,0,1,0
B	20	3,3,3,2,4,3,3,2,3,2,4,4,2,4,3,2,3,2,4,4

Appendix B

Bayes factor numerical results

Table B.1: Auckland data: averaged Bayes factors and associated posterior probabilities (P_i denotes $P(M_i \mid \boldsymbol{x})$) for the four competing models.

	Averaged Bayes factors						Posterior prob.			
Site	B^A_{21}	B^A_{31}	B^A_{41}	B^A_{32}	B^A_{42}	B^A_{43}	P_1	P_2	P_3	P_4
1	1.055	0.721	0.149	0.684	0.141	0.206	0.342	0.361	0.247	0.051
2	0.872	0.642	0.001	0.736	0.001	0.002	0.398	0.347	0.255	0.000
3	2.914	1.573	0.004	0.540	0.001	0.002	0.182	0.531	0.287	0.001
4	1.171	0.758	0.013	0.648	0.011	0.017	0.340	0.398	0.258	0.004
5	0.788	0.591	0.093	0.749	0.118	0.157	0.405	0.319	0.239	0.038
6	0.419	0.334	1E–5	0.799	2E–5	3E–5	0.571	0.239	0.191	0.000
7	0.799	0.577	0.031	0.721	0.039	0.054	0.416	0.332	0.240	0.013
8	0.992	0.729	0.276	0.735	0.278	0.378	0.334	0.331	0.243	0.092
9	3.133	2.165	1.322	0.691	0.422	0.611	0.131	0.411	0.284	0.174
10	438.0	417.3	2,655	0.953	6.061	6.362	0.000	0.125	0.119	0.756
11	0.808	0.598	0.035	0.741	0.044	0.059	0.409	0.331	0.245	0.015
12	0.810	0.607	0.067	0.749	0.082	0.110	0.403	0.326	0.244	0.027
13	3.260	1.944	4.678	0.597	1.435	2.406	0.092	0.300	0.179	0.430
14	0.711	0.574	0.052	0.808	0.073	0.090	0.428	0.304	0.246	0.022
15	0.869	0.672	0.097	0.774	0.112	0.144	0.379	0.329	0.255	0.037
16	0.762	0.604	0.115	0.793	0.150	0.190	0.403	0.307	0.244	0.046
17	0.514	0.431	0.002	0.839	0.004	0.004	0.514	0.264	0.222	0.001
18	2.432	1.834	4.066	0.754	1.672	2.217	0.107	0.261	0.197	0.436
19	0.900	0.695	0.326	0.772	0.362	0.469	0.342	0.308	0.238	0.112
20	0.608	0.504	0.016	0.830	0.026	0.032	0.470	0.286	0.237	0.008
21	0.847	0.653	0.066	0.771	0.078	0.101	0.390	0.330	0.255	0.026
22	0.785	0.652	0.261	0.831	0.333	0.401	0.371	0.291	0.242	0.097
23	3.070	1.851	5.221	0.603	1.701	2.821	0.090	0.276	0.166	0.469
24	1.054	0.819	0.406	0.778	0.385	0.495	0.305	0.321	0.250	0.124
25	1.231	0.877	0.412	0.712	0.335	0.470	0.284	0.350	0.249	0.117
26	0.750	0.625	0.137	0.833	0.182	0.219	0.398	0.299	0.249	0.054
27	0.790	0.672	0.345	0.851	0.437	0.513	0.356	0.281	0.239	0.123
28	0.645	0.591	0.143	0.917	0.221	0.241	0.420	0.271	0.249	0.060
29	0.862	0.711	0.442	0.825	0.513	0.621	0.332	0.286	0.236	0.147
30	0.692	0.675	0.261	0.975	0.378	0.387	0.380	0.263	0.257	0.099
31	17.42	7.481	27.01	0.430	1.551	3.611	0.019	0.329	0.141	0.511
32	2.087	1.433	2.830	0.687	1.356	1.975	0.136	0.284	0.195	0.385
33	1.237	0.932	1.202	0.754	0.972	1.290	0.229	0.283	0.213	0.275
34	0.872	0.755	0.571	0.866	0.655	0.757	0.313	0.273	0.236	0.179
35	0.997	0.826	0.891	0.829	0.894	1.079	0.269	0.268	0.222	0.240

Table B.2: Auckland data: approximated BIC Bayes factors and associated posterior probabilities (P_i denotes $P(M_i \mid x)$) for the four competing models.

	approximated BIC Bayes factors						Posterior prob.			
Site	B^S_{21}	B^S_{31}	B^S_{41}	B^S_{32}	B^S_{42}	B^S_{43}	P_1	P_2	P_3	P_4
1	0.464	0.216	0.111	0.465	0.240	0.516	0.558	0.259	0.121	0.062
2	0.228	0.100	0.001	0.437	0.003	0.008	0.753	0.172	0.075	0.001
3	1.041	0.246	0.003	0.236	0.003	0.012	0.437	0.455	0.107	0.001
4	0.324	0.083	0.010	0.257	0.031	0.121	0.706	0.229	0.059	0.007
5	0.408	0.167	0.081	0.408	0.198	0.484	0.604	0.247	0.101	0.049
6	0.213	0.046	1E–5	0.213	5E–5	2E–4	0.795	0.169	0.036	0.000
7	0.277	0.077	0.026	0.278	0.092	0.331	0.725	0.201	0.056	0.019
8	0.352	0.131	0.225	0.374	0.641	1.714	0.585	0.206	0.077	0.132
9	1.209	0.487	1.028	0.403	0.850	2.110	0.269	0.325	0.131	0.276
10	548.6	451.9	2,123	0.824	3.869	4.697	0.000	0.176	0.145	0.679
11	0.246	0.062	0.032	0.251	0.132	0.524	0.747	0.183	0.046	0.024
12	0.277	0.077	0.059	0.277	0.214	0.771	0.707	0.196	0.054	0.042
13	1.503	0.371	3.918	0.247	2.607	10.55	0.147	0.221	0.055	0.577
14	0.258	0.079	0.047	0.307	0.180	0.587	0.723	0.187	0.057	0.034
15	0.232	0.092	0.087	0.397	0.374	0.942	0.709	0.164	0.065	0.062
16	0.302	0.091	0.105	0.301	0.347	1.150	0.668	0.202	0.061	0.070
17	0.230	0.053	0.002	0.229	0.008	0.034	0.779	0.179	0.041	0.001
18	1.424	1.153	3.568	0.809	2.505	3.096	0.140	0.199	0.161	0.499
19	0.334	0.112	0.294	0.336	0.882	2.621	0.575	0.192	0.065	0.169
20	0.224	0.050	0.015	0.224	0.067	0.300	0.776	0.174	0.039	0.012
21	0.193	0.039	0.060	0.200	0.308	1.536	0.774	0.150	0.030	0.046
22	0.408	0.167	0.252	0.408	0.618	1.514	0.547	0.223	0.091	0.138
23	1.333	0.375	4.622	0.281	3.469	12.33	0.136	0.182	0.051	0.631
24	0.251	0.096	0.357	0.381	1.421	3.732	0.587	0.148	0.056	0.210
25	0.294	0.059	0.372	0.202	1.262	6.253	0.580	0.171	0.034	0.215
26	0.238	0.059	0.133	0.248	0.560	2.261	0.700	0.166	0.041	0.093
27	0.316	0.100	0.328	0.316	1.036	3.277	0.573	0.181	0.057	0.188
28	0.289	0.083	0.143	0.289	0.494	1.710	0.660	0.191	0.055	0.094
29	0.289	0.083	0.427	0.289	1.480	5.129	0.556	0.160	0.046	0.238
30	0.447	0.200	0.275	0.447	0.616	1.376	0.520	0.233	0.104	0.143
31	12.71	6.040	24.48	0.475	1.925	4.053	0.023	0.287	0.137	0.553
32	0.708	0.565	2.548	0.798	3.600	4.513	0.208	0.147	0.117	0.529
33	0.286	0.081	1.153	0.283	4.035	14.24	0.397	0.113	0.032	0.458
34	0.186	0.040	0.565	0.215	3.035	14.11	0.558	0.104	0.022	0.316
35	0.239	0.062	0.904	0.259	3.785	14.64	0.454	0.108	0.028	0.410

Appendix C

Tables of model adequacy and power calculations

Table C.1: Logged $d^i(M_1)$ measures and associated critical values for the *Poisson* model at the 35 accident sites using three separate discrepancy measures (listed with averaged Bayes factor rank). The symbols c^i and d^i denote $\log \widehat{c}^i_\alpha(M_1)$ and $\log d^i(M_1)$, respectively.

Site	Rank	d^1	c^1	d^2	c^2	d^3	c^3
1	2	2.3	(0.0, 2.8)	−15.0	(−18.1, −10.5)	−1.7	(−1.2)
2	1	3.3	(2.5, 3.7)	−53.3	(−58.0, −43.6)	−2.3	(−1.9)
3	3	4.0*	(2.9, 3.9)	−76.9	(−77.6, −61.0)	−2.6	(−2.1)
4	2	3.4	(2.4, 3.6)	−46.1	(−50.5, −36.5)	−2.1	(−1.9)
5	1	1.7	(0.0, 2.9)	−12.0	(−16.5, −8.9)	−2.1	(−1.3)
6	1	2.3*	(2.4, 3.7)	−36.2	(−49.0, −35.0)	−2.0	(−1.9)
7	1	2.6	(1.6, 3.3)	−24.4	(−30.1, −19.1)	−1.8	(−1.6)
8	1	2.4	(1.0, 3.1)	−18.0	(−21.8, −12.4)	−2.1	(−1.5)
9	4	3.7*	(2.4, 3.6)	−45.4	(−46.8, −32.6)	−1.6*	(−1.9)
10	4	4.3*	(1.8, 3.4)	−39.8*	(−32.9, −21.0)	−1.5*	(−1.7)
11	1	3.0	(2.0, 3.5)	−30.1	(−36.2, −23.4)	−3.3	(−1.8)
12	1	2.7	(1.6, 3.3)	−22.7	(−28.4, −17.0)	−2.2	(−1.7)
13	4	3.5*	(2.0, 3.5)	−34.5	(−35.5, −22.8)	−2.0	(−1.8)
14	1	2.6	(1.8, 3.4)	−25.7	(−31.7, −19.8)	−2.3	(−1.8)
15	1	3.1	(2.3, 3.6)	−34.7	(−40.3, −26.3)	−2.6	(−1.9)
16	1	2.3	(1.3, 3.2)	−18.5	(−23.8, −13.1)	−3.2	(−1.6)
17	1	2.4	(2.2, 3.6)	−28.2	(−38.2, −24.3)	−2.0	(−1.9)
18	4	3.3*	(0.4, 3.0)	−15.4	(−16.2, −7.2)	−1.7	(−1.4)
19	1	2.4	(1.0, 3.1)	−15.3	(−19.6, −9.8)	−3.5	(−1.5)
20	1	2.8	(2.3, 3.6)	−30.4	(−38.5, −24.3)	−2.9	(−1.9)
21	1	3.5	(2.8, 3.9)	−45.2	(−52.6, −35.1)	−3.2	(−2.1)
22	1	1.6	(0.0, 3.2)	−9.1	(−14.0, −5.1)	−2.3	(−1.3)
23	4	3.6*	(2.0, 3.5)	−28.4	(−30.6, −17.4)	−2.3	(−1.8)
24	2	3.3	(2.4, 3.7)	−34.4	(−40.1, −24.5)	−2.5	(−2.0)
25	2	3.6	(2.7, 3.8)	−42.1	(−48.0, −30.6)	−3.0	(−2.1)
26	1	2.9	(2.0, 3.5)	−23.3	(−30.4, −15.8)	−2.8	(−1.9)
27	1	2.1	(1.2, 3.3)	−13.0	(−18.7, −6.9)	−2.5	(−1.7)
28	1	2.0	(1.6, 3.4)	−14.0	(−21.1, −8.1)	−2.3	(−1.8)
29	1	2.6	(1.6, 3.4)	−15.4	(−21.2, −8.1)	−2.9	(−1.8)
30	1	0.0	(−0.7, 3.2)	−5.6	(−10.8, −0.6)	−1.4	(−1.3)
31	4	4.0*	(2.0, 3.6)	−24.2	(−26.2, −11.5)	−1.5*	(−1.9)
32	4	3.2	(1.8, 3.5)	−18.6	(−23.2, −8.6)	−1.8*	(−1.9)
33	3	3.4	(2.5, 3.8)	−25.4	(−32.6, −14.5)	−2.7	(−2.2)
34	1	3.4	(2.9, 4.0)	−28.7	(−38.5, −16.4)	−3.4	(−2.4)
35	1	3.1	(2.3, 3.8)	−17.4	(−25.4, −7.5)	−3.3	(−2.3)

Note: * denotes *inadequacy* at $\alpha = 0.05$.

Table C.2: Logged $d^i(M_1)$ measures and associated critical values for the *Poisson/gamma* model at the 35 accident sites using three separate discrepancy measures (listed with averaged Bayes factor rank). The symbols c^i and d^i denote $\log \widehat{c}^i_\alpha(M_1)$ and $\log d^i(M_1)$, respectively.

Site	Rank	d^1	c^1	d^2	c^2	d^3	c^3
1	1	1.9	(−0.1, 2.7)	−14.9	(−19.7, −10.7)	−1.8	(−1.3)
2	2	3.1	(2.5, 3.5)	−53.4	(−62.3, −44.8)	−2.5	(−2.0)
3	1	3.7	(3.1, 3.8)	−75.9	(−85.1, −63.4)	−3.0	(−2.1)
4	1	3.2	(2.4, 3.5)	−45.9	(−54.0, −37.4)	−2.3	(−1.9)
5	2	1.4	(−0.1, 2.8)	−12.2	(−18.2, −8.9)	−2.0	(−1.3)
6	2	2.2*	(2.3, 3.4)	−36.7	(−49.6, −35.8)	−1.9*	(−2.0)
7	2	2.4	(1.5, 3.1)	−24.6	(−32.0, −19.1)	−1.9	(−1.7)
8	2	2.1	(0.9, 3.0)	−18.0	(−23.8, −13.1)	−2.4	(−1.5)
9	1	3.3	(2.5, 3.7)	−44.2	(−52.5, −33.3)	−2.0*	(−2.0)
10	2	3.7	(2.3, 4.3)	−32.6	(−41.1, −19.4)	−2.1	(−1.7)
11	2	2.8	(2.0, 3.3)	−30.3	(−38.2, −23.6)	−3.0	(−1.8)
12	2	2.5	(1.5, 3.1)	−22.8	(−30.3, −17.4)	−2.3	(−1.7)
13	2	3.1	(2.1, 3.7)	−33.4	(−41.1, −21.7)	−2.8	(−1.8)
14	2	2.4	(1.8, 3.2)	−26.0	(−34.0, −20.0)	−2.3	(−1.8)
15	2	2.9	(2.3, 3.5)	−34.9	(−42.9, −26.8)	−2.4	(−2.0)
16	2	2.1	(1.3, 3.1)	−18.7	(−25.4, −13.7)	−2.8	(−1.7)
17	2	2.3	(2.2, 3.3)	−28.5	(−39.4, −24.8)	−1.9	(−1.8)
18	2	2.9	(0.6, 3.6)	−14.4	(−19.8, −6.5)	−1.9	(−1.4)
19	2	2.0	(0.9, 3.2)	−15.4	(−22.6, −9.7)	−3.0	(−1.5)
20	2	2.6	(2.2, 3.4)	−30.7	(−39.8, −24.6)	−2.8	(−1.9)
21	2	3.3	(2.8, 3.7)	−45.3	(−55.0, −35.5)	−3.6	(−2.2)
22	2	1.2	(−0.1, 2.8)	−9.3	(−15.6, −5.2)	−2.1	(−1.4)
23	2	3.2	(2.1, 3.9)	−27.4	(−35.1, −16.7)	−3.0	(−1.8)
24	1	3.0	(2.5, 3.6)	−34.4	(−42.6, −24.4)	−3.0	(−2.1)
25	1	3.4	(2.7, 3.7)	−42.0	(−53.1, −30.4)	−3.6	(−2.2)
26	2	2.7	(2.0, 3.4)	−23.5	(−32.6, −16.0)	−2.7	(−1.9)
27	2	1.8	(1.1, 3.3)	−13.2	(−20.1, −7.6)	−2.3	(−1.7)
28	2	1.8	(1.4, 3.2)	−14.4	(−22.6, −8.9)	−2.3	(−1.9)
29	2	2.3	(1.4, 3.3)	−15.5	(−23.3, −8.2)	−2.7	(−1.8)
30	2	−0.3*	(−0.3, 2.8)	−5.9	(−11.8, −1.0)	−1.4	(−1.3)
31	2	3.1	(2.1, 5.0)	−21.0	(−35.2, −7.1)	−2.5	(−1.6)
32	2	2.4	(1.8, 4.0)	−18.0	(−27.3, −6.9)	−2.3	(−1.8)
33	1	3.1	(2.5, 3.8)	−25.3	(−36.7, −13.5)	−3.3	(−2.2)
34	2	3.2	(2.8, 4.0)	−28.9	(−40.4, −17.1)	−3.5	(−2.5)
35	2	2.8	(2.2, 4.0)	−17.5	(−27.8, −7.5)	−3.7	(−2.2)

Note: * denotes *inadequacy* at $\alpha = 0.05$.

Table C.3: Logged $d^i(M_1)$ measures and associated critical values for the *mixture of two Poisson distributions* model at the 35 accident sites using three separate discrepancy measures (listed with averaged Bayes factor rank). The symbols c^i and d^i denote $\log \widehat{c}^i_\alpha(M_1)$ and $\log d^i(M_1)$, respectively.

Site	Rank	d^1	c^1	d^2	c^2	d^3	c^3
1	3	0.5	(−1.4, 2.2)	−15.1	(−21.0, −10.8)	−1.8	(−1.3)
2	3	2.8	(1.9, 3.4)	−53.4	(−61.5, −44.9)	−2.6	(−2.0)
3	2	3.6	(2.6, 3.7)	−76.3	(−84.6, −62.9)	−3.0	(−2.2)
4	3	2.8	(1.7, 3.3)	−46.1	(−54.6, −37.4)	−2.3	(−2.0)
5	3	−0.3	(−1.5, 2.2)	−12.3	(−19.6, −9.0)	−2.0	(−1.3)
6	3	1.4*	(1.6, 3.2)	−36.6	(−51.4, −35.6)	−1.9*	(−1.9)
7	3	1.4	(0.3, 2.7)	−24.7	(−32.7, −19.4)	−2.0	(−1.7)
8	3	0.9	(−0.6, 2.4)	−18.1	(−24.3, −12.6)	−2.4	(−1.5)
9	2	3.1	(1.7, 3.4)	−44.3	(−52.0, −33.9)	−2.0	(−1.9)
10	3	3.3	(1.0, 3.6)	−32.9	(−41.1, −18.7)	−2.4	(−1.8)
11	3	2.0	(0.9, 3.0)	−30.4	(−40.1, −23.8)	−3.0	(−1.8)
12	3	1.4	(0.2, 2.8)	−22.9	(−32.2, −17.1)	−2.3	(−1.7)
13	3	2.8	(1.1, 3.2)	−33.9	(−39.8, −23.0)	−2.7	(−1.9)
14	3	1.5	(0.6, 2.9)	−26.0	(−34.4, −19.9)	−2.3	(−1.8)
15	3	2.3	(1.3, 3.2)	−34.8	(−42.6, −26.5)	−2.4	(−2.0)
16	3	0.8	(−0.2, 2.6)	−18.7	(−26.4, −13.3)	−2.9	(−1.6)
17	3	1.4	(1.1, 3.1)	−28.5	(−40.8, −24.7)	−1.9	(−1.8)
18	3	1.2	(−1.3, 2.5)	−14.6	(−20.2, −6.0)	−1.9	(−1.4)
19	3	0.6	(−0.8, 2.4)	−15.4	(−22.8, −9.8)	−3.0	(−1.5)
20	3	1.8	(1.2, 3.2)	−30.7	(−41.3, −24.4)	−2.8	(−1.9)
21	3	2.9	(2.0, 3.6)	−45.4	(−55.1, −35.0)	−3.5	(−2.1)
22	3	−0.7	(−1.7, 2.1)	−9.4	(−17.5, −4.9)	−2.7	(−1.3)
23	3	2.6	(0.7, 3.1)	−27.9	(−34.8, −16.5)	−2.9	(−1.9)
24	3	2.6	(1.4, 3.3)	−34.4	(−42.6, −24.3)	−3.0	(−2.0)
25	3	3.0	(1.9, 3.5)	−42.0	(−51.4, −30.5)	−3.5	(−2.1)
26	3	1.7	(0.7, 2.9)	−23.5	(−33.2, −16.1)	−2.7	(−1.9)
27	3	0.3	(−0.8, 2.4)	−13.2	(−21.5, −6.7)	−2.4	(−1.7)
28	3	0.3	(−0.4, 2.6)	−14.3	(−23.5, −8.1)	−2.2	(−1.7)
29	3	1.0	(−0.5, 2.6)	−15.5	(−23.6, −7.7)	−2.8	(−1.8)
30	3	−2.0	(−2.1, 1.9)	−5.8	(−14.5, −1.7)	−1.4	(−1.3)
31	3	2.9	(0.1, 3.4)	−21.7	(−31.6, −8.4)	−2.3	(−1.9)
32	3	2.0	(−0.2, 2.9)	−18.0	(−26.8, −8.3)	−2.2	(−1.9)
33	4	2.5	(0.8, 3.3)	−25.4	(−34.9, −13.5)	−3.2	(−2.1)
34	3	2.7	(1.2, 3.5)	−28.8	(−40.5, −17.1)	−3.6	(−2.2)
35	4	1.9	(−0.2, 3.0)	−17.4	(−27.4, −7.5)	−3.4	(−2.0)

Note: * denotes *inadequacy* at $\alpha = 0.05$.

Table C.4: Logged $d^i(M_1)$ measures and associated critical values for the *geometric* model at the 35 accident sites using three separate discrepancy measures (listed with averaged Bayes factor rank). The symbols c^i and d^i denote $\log \widehat{c}^i_\alpha(M_1)$ and $\log d^i(M_1)$, respectively.

Site	Rank	d^1	c^1	d^2	c^2	d^3	c^3
1	4	0.0	(−0.5, 3.4)	−16.6	(−24.1, −9.8)	−1.2	(−1.0)
2	4	1.6*	(2.3, 4.0)	−60.0	(−73.9, −46.8)	−1.4*	(−1.7)
3	4	2.3*	(2.8, 4.2)	−82.1	(−98.8, −66.3)	−1.4*	(−1.9)
4	4	1.9*	(2.2, 4.0)	−50.2	(−64.0, −37.4)	−1.6*	(−1.7)
5	4	−0.2	(−0.5, 3.5)	−14.2	(−21.9, −7.6)	−1.4	(−1.1)
6	4	0.9*	(2.2, 4.0)	−47.6	(−61.4, −35.0)	−1.1*	(−1.7)
7	4	1.2*	(1.3, 3.7)	−27.7	(−38.2, −18.1)	−1.3*	(−1.5)
8	4	0.9	(0.5, 3.6)	−19.1	(−28.0, −10.9)	−1.7	(−1.3)
9	3	2.4	(2.2, 4.0)	−44.7	(−58.1, −31.9)	−1.8	(−1.7)
10	1	3.1	(1.5, 3.8)	−30.7	(−41.4, −19.6)	−2.0	(−1.6)
11	4	1.7*	(1.8, 3.9)	−33.2	(−44.9, −22.3)	−1.5*	(−1.6)
12	4	1.4	(1.3, 3.8)	−25.1	(−35.7, −15.7)	−1.3*	(−1.5)
13	1	2.4	(1.8, 3.8)	−32.5	(−44.2, −21.1)	−2.4	(−1.6)
14	4	1.3*	(1.5, 3.8)	−28.5	(−39.7, −17.9)	−1.8	(−1.6)
15	4	2.0*	(2.0, 3.9)	−36.8	(−49.8, −24.8)	−1.7*	(−1.7)
16	4	1.0	(0.9, 3.7)	−20.4	(−30.3, −11.4)	−1.7	(−1.4)
17	4	1.3*	(2.0, 3.9)	−34.3	(−47.1, −22.5)	−1.2*	(−1.7)
18	1	2.1	(−0.2, 3.6)	−13.2	(−20.7, −5.7)	−2.1	(−1.2)
19	4	1.1	(0.5, 3.7)	−16.2	(−25.1, −8.0)	−1.8	(−1.4)
20	4	1.7*	(2.0, 4.0)	−34.3	(−47.2, −22.1)	−1.6*	(−1.8)
21	4	2.5*	(2.6, 4.1)	−47.7	(−62.8, −33.1)	−2.0*	(−2.0)
22	4	0.2	(−0.6, 3.6)	−10.3	(−17.9, −4.0)	−1.4	(−1.2)
23	1	2.6	(1.7, 3.9)	−26.3	(−37.6, −15.2)	−2.8	(−1.7)
24	4	2.3	(2.2, 4.0)	−35.1	(−48.6, −22.1)	−2.5	(−1.8)
25	4	2.7	(2.5, 4.1)	−42.7	(−57.2, −28.5)	−2.2	(−1.9)
26	4	2.0	(1.8, 3.9)	−25.0	(−36.6, −14.1)	−1.7*	(−1.8)
27	4	1.1	(0.8, 3.8)	−13.9	(−23.2, −6.3)	−2.0	(−1.5)
28	4	1.1*	(1.1, 3.8)	−15.9	(−26.0, −6.7)	−1.6*	(−1.6)
29	4	1.8	(1.1, 3.8)	−16.0	(−25.9, −6.7)	−2.1	(−1.6)
30	4	−1.1*	(−1.0, 3.1)	−6.8	(−13.8, −0.6)	−1.1*	(−1.2)
31	1	3.4	(1.7, 3.9)	−20.5	(−31.2, −9.2)	−2.1	(−1.8)
32	1	2.5	(1.4, 4.0)	−17.3	(−27.6, −7.0)	−2.4	(−1.8)
33	2	2.8	(2.2, 4.1)	−25.0	(−38.2, −12.3)	−3.5	(−2.0)
34	4	2.9	(2.6, 4.2)	−29.1	(−44.1, −15.1)	−3.0	(−2.3)
35	3	2.7	(2.0, 4.1)	−17.3	(−29.2, −5.1)	−3.3	(−2.1)

Note: * denotes *inadequacy* at $\alpha = 0.05$.

Table C.5: Power (%) at $\alpha = 0.05$ to detect model inadequacy using each of the three adequacy measures when the *Poisson* distribution was actually generating the data. The symbol $P^r_{j|1}$ denotes $\widehat{P}^r(M_j, M_1)$.

Site	$P^1_{2\|1}$	$P^2_{2\|1}$	$P^3_{2\|1}$	$P^1_{3\|1}$	$P^2_{3\|1}$	$P^3_{3\|1}$	$P^1_{4\|1}$	$P^2_{4\|1}$	$P^3_{4\|1}$
1	4	3	8	2	3	7	56	0	50
2	5	4	8	2	6	7	100	0	98
3	11	7	6	1	6	9	100	0	100
4	5	4	5	2	5	9	97	0	93
5	3	2	6	1	2	6	38	0	35
6	4	6	7	5	4	7	94	0	89
7	3	2	5	2	3	7	69	0	63
8	4	3	6	3	2	8	47	0	42
9	9	3	7	0	4	9	88	0	83
10	33	0	4	0	0	11	69	0	60
11	3	3	6	3	2	7	72	0	64
12	4	3	6	3	3	7	56	0	49
13	10	1	5	1	2	11	68	0	61
14	3	2	6	4	3	7	61	0	55
15	4	4	6	3	2	9	72	0	65
16	5	5	7	4	2	6	45	0	40
17	5	3	6	5	3	6	67	0	60
18	5	1	3	1	1	11	19	1	24
19	4	3	7	3	3	9	29	0	32
20	4	3	5	4	2	7	63	0	59
21	5	3	8	4	3	7	77	0	71
22	5	3	7	3	2	9	13	2	20
23	10	2	5	1	1	9	44	1	42
24	7	2	9	5	3	7	59	0	53
25	4	2	7	4	2	9	66	0	60
26	4	4	6	10	3	7	37	1	33
27	4	7	4	8	2	9	15	2	19
28	4	4	7	9	3	7	19	2	22
29	3	4	5	11	2	8	19	1	22
30	7	5	7	4	4	7	13	5	13
31	13	0	0	1	1	6	24	1	25
32	5	1	2	6	3	10	19	1	20
33	5	3	3	9	2	8	26	1	24
34	4	4	5	13	4	6	24	2	22
35	6	5	3	19	3	7	14	2	11

Table C.6: Power (%) at $\alpha = 0.05$ to detect model inadequacy using each of the three adequacy measures when the *Poisson/gamma* distribution was actually generating the data. The symbol $P^r_{j|2}$ denotes $\widehat{P}^r(M_j, M_2)$.

Site	$P^1_{1\|2}$	$P^2_{1\|2}$	$P^3_{1\|2}$	$P^1_{3\|2}$	$P^2_{3\|2}$	$P^3_{3\|2}$	$P^1_{4\|2}$	$P^2_{4\|2}$	$P^3_{4\|2}$
1	12	14	8	4	3	5	42	0	39
2	16	16	10	5	5	4	96	0	93
3	34	31	20	7	6	5	95	0	93
4	19	17	12	5	5	5	84	0	79
5	9	11	7	3	3	4	31	0	29
6	6	7	6	3	4	5	91	0	84
7	10	12	7	4	4	4	56	0	52
8	12	14	9	5	6	6	35	1	33
9	30	26	21	7	7	5	53	1	51
10	61	52	48	6	7	4	13	4	12
11	12	12	8	4	4	4	58	0	52
12	11	11	8	3	3	5	43	1	40
13	32	27	22	8	7	5	32	1	30
14	11	12	9	5	4	6	50	0	46
15	13	12	9	6	5	6	56	1	51
16	10	11	8	4	5	4	35	0	32
17	8	8	7	4	3	5	59	0	53
18	19	22	14	4	3	5	10	3	13
19	10	13	9	4	4	5	22	1	25
20	10	9	7	3	4	4	53	0	51
21	12	12	10	4	5	6	60	1	56
22	8	11	6	3	3	5	10	2	17
23	25	23	20	6	6	3	20	2	21
24	15	14	11	6	6	4	40	1	38
25	17	15	13	8	5	5	44	1	41
26	9	10	8	5	5	4	28	1	26
27	9	13	9	4	4	5	12	3	16
28	8	10	7	4	4	4	16	2	18
29	10	11	9	4	4	5	14	2	17
30	11	11	8	3	3	6	11	5	11
31	43	35	37	11	8	5	14	9	14
32	19	19	17	8	7	5	11	5	13
33	15	14	14	7	6	5	16	3	17
34	13	10	12	7	7	5	17	3	16
35	10	11	13	7	6	5	10	3	9

Table C.7: Power (%) at $\alpha = 0.05$ to detect model inadequacy using each of the three adequacy measures when the *mixture of two Poisson distributions* model was actually generating the data. The symbol $P^r_{j|3}$ denotes $\widehat{P}^r(M_j, M_3)$.

Site	$P^1_{1\|3}$	$P^2_{1\|3}$	$P^3_{1\|3}$	$P^1_{2\|3}$	$P^2_{2\|3}$	$P^3_{2\|3}$	$P^1_{4\|3}$	$P^2_{4\|3}$	$P^3_{4\|3}$
1	16	17	12	6	7	8	41	1	38
2	18	17	12	5	3	6	95	0	91
3	31	29	21	8	6	7	95	0	95
4	19	17	13	5	6	7	85	0	80
5	13	15	11	6	8	7	31	2	30
6	10	10	8	7	8	9	89	1	84
7	12	13	9	7	7	6	57	1	53
8	14	15	12	7	8	7	36	2	34
9	34	30	26	3	5	7	50	1	49
10	74	68	61	7	7	15	12	5	17
11	12	12	10	7	6	5	61	2	55
12	12	13	10	8	7	7	44	2	41
13	27	24	21	5	2	6	36	1	33
14	11	12	10	8	6	8	51	2	47
15	12	11	10	5	7	7	58	1	53
16	11	12	9	6	9	8	37	2	33
17	9	9	8	10	7	8	62	1	56
18	24	28	20	7	6	8	11	4	14
19	12	14	10	5	6	6	24	2	27
20	10	10	8	7	7	8	55	2	52
21	11	11	9	6	6	9	64	1	58
22	11	14	9	7	10	9	11	4	18
23	24	23	19	6	6	5	22	2	23
24	12	13	11	6	7	9	43	1	39
25	15	13	11	5	3	6	47	1	44
26	10	10	8	6	6	7	30	2	28
27	9	13	9	6	8	7	13	4	17
28	9	11	8	7	8	8	16	3	19
29	10	11	9	7	7	5	16	4	19
30	14	13	11	13	20	8	13	8	13
31	39	30	37	4	3	2	10	6	13
32	15	16	16	4	5	5	12	4	14
33	11	11	11	6	5	6	18	3	17
34	9	8	9	4	6	6	19	3	17
35	8	9	9	5	9	4	11	5	9

Table C.8: Power (%) at $\alpha = 0.05$ to detect model inadequacy using each of the three adequacy measures when the *geometric* model was actually generating the data. The symbol $P^r_{j|4}$ denotes $\widehat{P}^r(M_j, M_4)$.

Site	$P^1_{1\|4}$	$P^2_{1\|4}$	$P^3_{1\|4}$	$P^1_{2\|4}$	$P^2_{2\|4}$	$P^3_{2\|4}$	$P^1_{3\|4}$	$P^2_{3\|4}$	$P^3_{3\|4}$
1	71	70	52	30	40	11	33	29	2
2	99	93	95	36	46	11	70	58	10
3	100	96	99	28	38	9	68	58	17
4	96	85	88	26	35	6	59	41	6
5	57	59	41	24	37	7	21	23	1
6	93	80	85	45	47	12	79	44	4
7	76	67	62	33	32	8	48	31	2
8	62	58	48	22	29	7	33	27	3
9	90	73	80	16	17	9	31	26	4
10	76	64	63	4	7	5	5	9	4
11	79	63	64	33	30	7	43	24	2
12	68	57	53	32	29	9	33	20	2
13	76	61	62	11	13	7	25	23	4
14	71	60	58	31	25	9	43	27	3
15	78	60	64	25	26	9	40	30	3
16	56	52	43	24	29	9	28	23	2
17	75	59	63	40	32	6	48	28	2
18	40	43	30	7	12	5	7	11	3
19	45	47	35	16	19	7	17	18	2
20	72	54	58	30	33	8	39	26	2
21	79	55	68	29	24	7	44	27	2
22	30	40	22	19	23	11	8	13	3
23	54	46	45	5	12	5	15	15	3
24	65	48	52	17	20	10	33	23	2
25	72	50	61	22	16	8	36	20	4
26	48	40	39	18	18	8	27	17	2
27	27	36	26	11	20	6	12	13	3
28	30	32	25	16	21	11	14	15	3
29	31	31	25	13	18	6	14	14	3
30	25	29	16	13	20	8	5	8	4
31	32	29	29	2	2	0	3	5	2
32	27	28	25	4	8	3	9	10	4
33	32	25	30	11	9	9	14	13	4
34	33	23	32	8	13	9	21	14	6
35	16	19	21	6	10	7	12	9	7

Appendix D

Simulation hints and tables of predictive probability calculations

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The uniform, 'shoe' and exponential distributions were easily generated by the inverse transformation method, as described in Pidd (1986) and briefly summarised in Section 4.6.3.

Gamma distributed variants can readily be generated from an algorithm detailed in Fishman (1973), and briefly described as follows. Suppose that X is from a gamma distribution, $g(a,b)$, and $k = [a]$ where the quantity $[a]$ denotes the largest integer in a. Fishman considered X to be the sum of $k+1$ independent gamma variants, all with scale parameter b, but the first k of which have unit shape parameter and the $k+1^{th}$ having shape parameter $y = a - [a]$. If Y and Z are independent variants from $\mathcal{B}e(\gamma, 1-\gamma)$ (the beta density) and $g(1,1)$, which is the $\mathcal{E}(1)$ (the exponential density), respectively. Then $W = (1/b)YZ$ is a variate with $g(a,b)$.

Generations from both $\mathcal{B}e(\gamma, 1-\gamma)$ and $\mathcal{E}(1)$ distributions are straightforward;

$$Y = \frac{U_1[0,1]^{1/\gamma}}{U_1[0,1]^{1/\gamma} + U_2[0,1]^{1/(1-\gamma)}} \quad \text{and}$$

$$Z = -\log(U[0,1])$$

provided $U_1[0,1]^{1/\gamma} + U_2[0,1]^{1/(1-\gamma)} \leq 1$, where $U_i[0,1]$ is a random variate from the uniform $[0,1]$ distribution, $\mathcal{U}(0,1)$.

For the posterior probabilities numerical calculations of the cumulative gamma distribution required determination. The cumulative two parameter gamma density can be rewritten as

$$\begin{aligned} G(x \mid a,b) &= \int_0^x g(u \mid a,b)\, du \quad \text{for } a>0,\ b>0 \\ &= \int_0^x \frac{b(bu)^{a-1}}{\Gamma(a)} e^{-bu}\, du \\ &= \frac{1}{\Gamma(a)} \int_0^{bx} t^{a-1} e^{-t}\, dt. \end{aligned}$$

Bowman and Shenton (1988) describe at least three methods in which this form of $G(x \mid a,b)$ can be numerically computed; expanding the exponential, the Stieltjies continued fraction approach and the continued fraction of Schlomilch. The latter of these approaches is most readily adopted for these calculations, where

$$\frac{1}{\Gamma(a)} \int_0^x t^{a-1} e^{-t}\, dt = \frac{e^{-x} x^a}{\Gamma(a)} \left(\frac{1}{a-x+} \frac{x}{a-x+1+} \frac{2x}{a-x+2+} \frac{3x}{a-x+3+} \cdots \right)$$

for $x > 0$ and $a > 0$. The gamma function was calculated via the asymptotic formula, such that

$$\begin{aligned} \ln \Gamma(x) \approx\ & (x-\frac{1}{2}) \ln x - x + \frac{1}{2} \ln 2\pi + \frac{1}{12x} - \frac{1}{360x^3} + \\ & \frac{1}{1260x^5} - \frac{1}{1680x^7} + \frac{1}{1188x^9} - \frac{691}{360360x^{11}} + \ldots \end{aligned} \tag{D.1}$$

which converges rapidly achieving any desired level of accuracy when x is large. If however x is small then implementation of the recurrence formula

$$\Gamma(x) = \frac{\Gamma(x+m)}{x\,(x+1)\ldots(x+m-1)} \quad \text{for } m = 1,2,\ldots$$

ensures that equation (D.1) converges rapidly for any x. The specified accuracy level was assigned to be $\pm$ 0.00001, which ordinarily could be reached in summing ten terms of the continued fraction.

Table D.1: Predictive probabilities, $pd_i(n_0)$, for information scenarios 1 and 2.

	Scenario 1, with $n_0 =$						Scenario 2, with $n_0 =$					
Site	0	1	2	3	4	5	0	1	2	3	4	5
1	1.00	.976	.891	.738	.547	.365	1.00	.974	.885	.728	.535	.350
2	1.00	.974	.881	.711	.506	.317	1.00	.974	.879	.708	.503	.313
3	1.00	.975	.883	.716	.510	.319	1.00	.975	.882	.714	.507	.317
4	1.00	.942	.780	.551	.332	.172	1.00	.941	.777	.546	.328	.169
5	1.00	.922	.734	.498	.291	.149	1.00	.920	.730	.492	.285	.144
6	1.00	.919	.719	.469	.259	.122	1.00	.919	.719	.469	.257	.121
7	1.00	.900	.676	.420	.220	.100	1.00	.900	.676	.419	.219	.099
8	1.00	.883	.643	.385	.195	.085	1.00	.882	.640	.384	.194	.085
9	1.00	.884	.638	.374	.183	.076	1.00	.883	.637	.373	.181	.075
10	1.00	.869	.611	.347	.166	.067	1.00	.869	.610	.348	.165	.067
11	1.00	.854	.581	.318	.144	.056	1.00	.855	.582	.317	.143	.055
12	1.00	.841	.560	.299	.132	.050	1.00	.843	.560	.300	.133	.050
13	1.00	.839	.552	.291	.127	.047	1.00	.839	.552	.290	.126	.047
14	1.00	.836	.548	.287	.124	.046	1.00	.836	.548	.287	.124	.046
15	1.00	.821	.519	.259	.106	.037	1.00	.820	.518	.258	.106	.037
16	1.00	.812	.511	.256	.106	.038	1.00	.814	.511	.256	.106	.038
17	1.00	.809	.500	.243	.097	.033	1.00	.810	.503	.245	.098	.033
18	1.00	.784	.472	.228	.092	.032	1.00	.786	.473	.229	.092	.032
19	1.00	.783	.466	.221	.087	.030	1.00	.786	.470	.224	.088	.030
20	1.00	.774	.447	.200	.073	.023	1.00	.778	.449	.202	.075	.023
21	1.00	.748	.408	.171	.057	.016	1.00	.751	.410	.171	.058	.017
22	1.00	.745	.417	.187	.071	.024	1.00	.750	.421	.189	.071	.024
23	1.00	.735	.394	.162	.055	.015	1.00	.738	.396	.164	.056	.016
24	1.00	.723	.376	.150	.048	.013	1.00	.727	.379	.151	.049	.014
25	1.00	.721	.371	.145	.046	.012	1.00	.722	.371	.146	.046	.012
26	1.00	.671	.313	.112	.032	.008	1.00	.673	.317	.114	.033	.008
27	1.00	.635	.281	.097	.028	.007	1.00	.642	.288	.101	.029	.007
28	1.00	.608	.252	.081	.021	.005	1.00	.615	.259	.084	.022	.005
29	1.00	.608	.253	.081	.021	.005	1.00	.615	.259	.084	.022	.005
30	1.00	.636	.292	.108	.034	.010	1.00	.647	.303	.113	.036	.010
31	1.00	.570	.216	.062	.014	.003	1.00	.576	.222	.065	.016	.003
32	1.00	.561	.211	.060	.014	.003	1.00	.568	.216	.063	.015	.003
33	1.00	.512	.170	.042	.009	.002	1.00	.518	.174	.043	.009	.002
34	1.00	.445	.124	.025	.004	.001	1.00	.452	.128	.027	.004	.001
35	1.00	.417	.109	.022	.004	.001	1.00	.426	.114	.022	.004	.001

Table D.2: Predictive probabilities, $pd_i(n_0)$, for information scenario 3 and using the quasi-noninformative scenario.

	Scenario 3, with $n_0 =$						Scenario non-info, with $n_0 =$					
Site	0	1	2	3	4	5	0	1	2	3	4	5
1	1.00	.973	.879	.715	.518	.334	1.00	.975	.890	.737	.546	.363
2	1.00	.973	.877	.705	.498	.310	1.00	.974	.880	.711	.507	.317
3	1.00	.741	.881	.711	.503	.313	1.00	.975	.883	.716	.510	.319
4	1.00	.941	.776	.545	.327	.169	1.00	.941	.779	.549	.331	.172
5	1.00	.918	.724	.485	.278	.140	1.00	.921	.732	.496	.290	.148
6	1.00	.919	.718	.466	.256	.120	1.00	.919	.720	.470	.259	.122
7	1.00	.898	.673	.415	.215	.097	1.00	.900	.676	.420	.220	.099
8	1.00	.882	.640	.381	.192	.083	1.00	.882	.641	.384	.194	.085
9	1.00	.882	.635	.372	.181	.075	1.00	.883	.637	.373	.182	.075
10	1.00	.870	.611	.347	.164	.067	1.00	.869	.610	.347	.165	.067
11	1.00	.855	.582	.318	.144	.055	1.00	.855	.580	.317	.143	.055
12	1.00	.843	.562	.300	.133	.050	1.00	.842	.559	.299	.131	.050
13	1.00	.841	.555	.292	.127	.047	1.00	.839	.552	.290	.124	.046
14	1.00	.837	.550	.289	.125	.046	1.00	.835	.547	.285	.123	.046
15	1.00	.821	.521	.261	.107	.037	1.00	.820	.518	.259	.106	.037
16	1.00	.816	.515	.259	.108	.039	1.00	.811	.510	.255	.106	.038
17	1.00	.812	.505	.247	.099	.033	1.00	.809	.500	.244	.096	.033
18	1.00	.792	.480	.234	.095	.033	1.00	.784	.470	.226	.092	.032
19	1.00	.790	.475	.227	.090	.031	1.00	.782	.465	.219	.086	.030
20	1.00	.779	.454	.204	.075	.023	1.00	.775	.447	.200	.073	.023
21	1.00	.752	.412	.173	.059	.017	1.00	.749	.408	.170	.057	.016
22	1.00	.757	.431	.197	.075	.025	1.00	.745	.416	.186	.070	.023
23	1.00	.742	.401	.168	.057	.017	1.00	.736	.393	.162	.055	.016
24	1.00	.730	.385	.155	.051	.014	1.00	.725	.377	.150	.048	.013
25	1.00	.725	.377	.149	.047	.012	1.00	.721	.370	.145	.045	.012
26	1.00	.680	.324	.118	.035	.009	1.00	.670	.312	.111	.032	.008
27	1.00	.653	.300	.107	.032	.008	1.00	.634	.280	.095	.027	.007
28	1.00	.627	.272	.090	.025	.006	1.00	.607	.252	.081	.021	.005
29	1.00	.627	.271	.090	.025	.006	1.00	.608	.252	.081	.021	.005
30	1.00	.667	.323	.124	.041	.012	1.00	.636	.291	.107	.034	.010
31	1.00	.588	.232	.069	.017	.004	1.00	.569	.216	.062	.014	.003
32	1.00	.581	.228	.068	.016	.003	1.00	.559	.209	.059	.014	.003
33	1.00	.529	.182	.046	.010	.002	1.00	.511	.168	.042	.008	.001
34	1.00	.463	.135	.029	.005	.001	1.00	.446	.125	.026	.004	.001
35	1.00	.443	.125	.026	.004	.001	1.00	.415	.110	.022	.004	.001